```
Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:ssptayvv1621

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  AUG 15  CAOLD to be discontinued on December 31, 2008
 NEWS  3  OCT 07  EPFULL enhanced with full implementation of EPC2000
 NEWS  4  OCT 07  Multiple databases enhanced for more flexible patent
                  number searching
 NEWS  5  OCT 22  Current-awareness alert (SDI) setup and editing
                  enhanced
 NEWS  6  OCT 22  WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT
                  Applications
 NEWS  7  OCT 24  CHEMLIST enhanced with intermediate list of
                  pre-registered REACH substances
 NEWS  8  NOV 21  CAS patent coverage to include exemplified prophetic
                  substances identified in English-, French-, German-,
                  and Japanese-language basic patents from 2004-present
 NEWS  9  NOV 26  MARPAT enhanced with FSORT command
 NEWS 10  NOV 26  MEDLINE year-end processing temporarily halts
                  availability of new fully-indexed citations
 NEWS 11  NOV 26  CHEMSAFE now available on STN Easy
 NEWS 12  NOV 26  Two new SET commands increase convenience of STN
                  searching
 NEWS 13  DEC 01  ChemPort single article sales feature unavailable
 NEWS 14  DEC 12  GBFULL now offers single source for full-text
                  coverage of complete UK patent families
 NEWS 15  DEC 17  Fifty-one pharmaceutical ingredients added to PS

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN Customer
  agreement.  Please note that this agreement limits use to scientific
  research.  Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:06:05 ON 19 DEC 2008

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
```

	ENTRY	SESSION
FULL ESTIMATED COST	0.42	0.42

FILE 'REGISTRY' ENTERED AT 16:06:57 ON 19 DEC 2008

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 18 DEC 2008 HIGHEST RN 1086785-80-9
DICTIONARY FILE UPDATES: 18 DEC 2008 HIGHEST RN 1086785-80-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

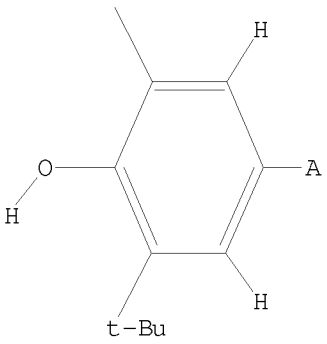
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10530572.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

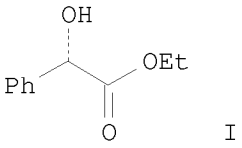
=> s l1
SAMPLE SEARCH INITIATED 16:07:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3773 TO ITERATE

53.0% PROCESSED 2000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

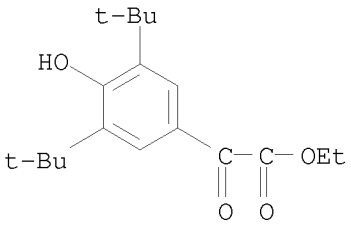
```
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        71776 TO    79144
PROJECTED ANSWERS:           18567 TO    22407

L2           50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 16:07:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    75664 TO ITERATE

100.0% PROCESSED    75664 ITERATIONS                          20171 ANSWERS
SEARCH TIME: 00.00.01

L3        20171 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     178.36     178.78

FILE 'CAPLUS' ENTERED AT 16:07:34 ON 19 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 19 Dec 2008  VOL 149 ISS 26
FILE LAST UPDATED: 18 Dec 2008  (20081218/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l3
L4        22946 L3

=> s l4 and chiral
         128631 CHIRAL
L5           40 L4 AND CHIRAL

=> d l5 ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 40 ANSWERS - CONTINUE? Y/(N):y

L5   ANSWER 1 OF 40  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2008:496195  CAPLUS
DOCUMENT NUMBER:          148:561527
TITLE:                    CeCl3·7H2O: An Effective Additive in
                          Ru-Catalyzed Enantioselective Hydrogenation of
                          Aromatic α-Ketoesters
```

AUTHOR(S): Meng, Qinghua; Sun, Yanhui; Ratovelomanana-Vidal, Virginie; Genet, Jean Pierre; Zhang, Zhaoguo
CORPORATE SOURCE: School of Chemistry and Chemical Technology, Shanghai Jiaotong University, Shanghai, 200240, Peop. Rep. China
SOURCE: Journal of Organic Chemistry (2008), 73(10), 3842-3847
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:561527
GI

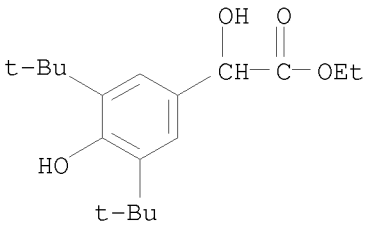


I

AB In the presence of catalytic amts. of CeCl3·7H2O, [RuCl(benzene)(S)-SunPhos]Cl is a highly effective catalyst for the asym. hydrogenation of aromatic α-ketoesters. A variety of Et α-hydroxy-α-arylacetates, e.g., I, have been prepared in up to 98.3% ee with a TON up to 10 000. Challenging aromatic α-ketoesters with ortho substituents are also hydrogenated with high enantioselectivities. The addition of CeCl3·7H2O not only improves the enantioselectivity but also enhances the stability of the catalyst. The ratio of CeCl3·7H2O to [RuCl(benzene)(S)-SunPhos]Cl plays an important role in the hydrogenation reaction with a large substrate/catalyst ratio.
IT 67739-25-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of Et α-hydroxy-α-arylacetates via in situ generated chiral Ru(SunPhos)/CeCl3 heptahydrate catalyzed hydrogenation of aromatic α-ketoesters)
RN 67739-25-7 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-oxo-, ethyl ester (CA INDEX NAME)



IT 1026130-72-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of Et α-hydroxy-α-arylacetates via in situ generated chiral Ru(SunPhos)/CeCl3 heptahydrate catalyzed hydrogenation of aromatic α-ketoesters)
RN 1026130-72-2 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-α,4-dihydroxy-, ethyl ester (CA INDEX NAME)

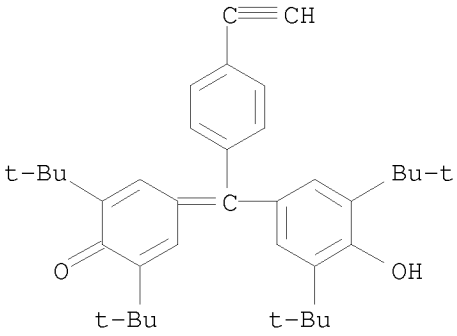


REFERENCE COUNT: 105 THERE ARE 105 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:958212 CAPLUS
DOCUMENT NUMBER: 147:486691
TITLE: Helix-Sense Tunability Induced by Achiral Diene Ligands in the Chiral Catalytic System for the Helix-Sense-Selective Polymerization of Achiral and Bulky Phenylacetylene Monomers
AUTHOR(S): Kaneko, Takashi; Umeda, Yasuhiro; Jia, Honge; Hadano, Shingo; Teraguchi, Masahiro; Aoki, Toshiki
CORPORATE SOURCE: Center for Transdisciplinary Research, and Graduate School of Science and Technology, and Venture Business Laboratory, and Department of Chemistry and Chemical Engineering, Faculty of Engineering, Niigata University, Niigata, 950-2181, Japan
SOURCE: Macromolecules (Washington, DC, United States) (2007), 40(20), 7098-7102
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Helix-sense-selective polymerization of {4-[(3,5-di-tert-butyl-4-hydroxyphenyl)(3,5-di-tert-butyl-4-oxo-cyclohexa-2,5-dienylidene)methyl]phenyl}acetylene (abbreviated as (4-ethynylphenyl)hydrogalvinoxyl) was promoted by [Rh(cod)Cl]2 and [Rh(nbd)Cl]2 catalyst in the presence of (R)-(+)-1-phenylethylamine or (S)-(-)-1-phenylethylamine (PEA). The [Rh(cod)Cl]2 catalyst system gave red polymers whose CD spectra showed the stronger Cotton effect though the yield (2-3%) and mol. weight (Mn=(1.1-1.4)+104) were lower than those of polymers obtained by [Rh(nbd)Cl]2. Moreover, we studied the effect of bulkiness of the catalyst, cocatalyst, and monomer on helix-sense-selective polymerization of (4-ethynylphenyl)hydrogalvinoxyl in the presence of (R)-PEA. The CD patterns of polymers obtained by [Rh(nbd)Cl]2 and [Rh(cod)Cl]2 were nearly mirror image of each other, except for the magnitudes of the signals in spite of the same chiral condition, i.e., in the presence of (R)-PEA. That is, [Rh(nbd)Cl]2 and [Rh(cod)Cl]2 catalysts generated P-helix and M-helix, resp. This is a novel result, since the control of helix sense is usually achieved by enantiomeric moieties of catalysts or initiators for the helix-sense-selective polymerization
IT 129217-05-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(effect of achiral diene ligands in chiral catalytic systems on helix-sense-selective polymerization of achiral and bulky phenylacetylene monomers)
RN 129217-05-6 CAPLUS
CN 2,5-Cyclohexadien-1-one, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl](4-ethynylphenyl)methylene]-2,6-bis(1,1-dimethylethyl)-, homopolymer (CA INDEX NAME)

CM 1

CRN 129216-99-5
CMF C37 H46 O2



REFERENCE COUNT: 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:640728 CAPLUS
DOCUMENT NUMBER: 147:72651
TITLE: Preparation of nitrogen-containing heteroaryl-substituted aryl bicycles as kinase inhibitors for the treatment of cancer
INVENTOR(S): Calderwood, Emily F.; Duffey, Matthew; Gould, Alexandra E.; Greenspan, Paul D.; Kulkarni, Bheemashankar; Lamarche, Matthew J.; Rowland, Robyn Scott; Tregay, Ming; Vos, Tricia J.
PATENT ASSIGNEE(S): Millennium Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 292pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

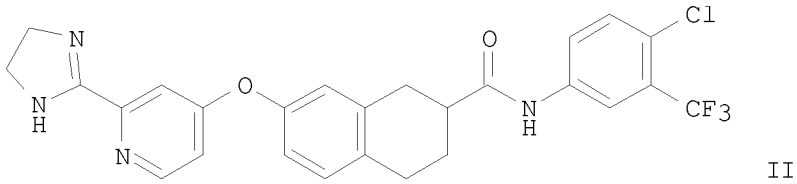
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007067444	A1	20070614	WO 2006-US46097	20061207
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2006322094	A1	20070614	AU 2006-322094	20061207
CA 2632512	A1	20070614	CA 2006-2632512	20061207
US 20070149533	A1	20070628	US 2006-636609	20061207
EP 1957460	A1	20080820	EP 2006-838840	20061207
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL,				

BA, HR, MK, RS

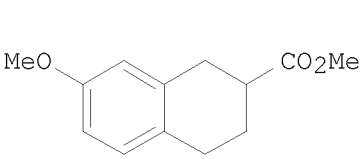
NO 2008002476	A	20080624	NO 2008-2476		20080529
MX 200807179	A	20080627	MX 2008-7179		20080605
IN 2008DN05257	A	20081024	IN 2008-DN5257		20080618
KR 2008074220	A	20080812	KR 2008-716456		20080707
PRIORITY APPLN. INFO.:			US 2005-748369P	P	20051208
			WO 2006-US46097	W	20061207

OTHER SOURCE(S): MARPAT 147:72651

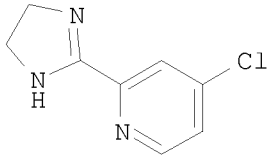
GI



II



III



IV

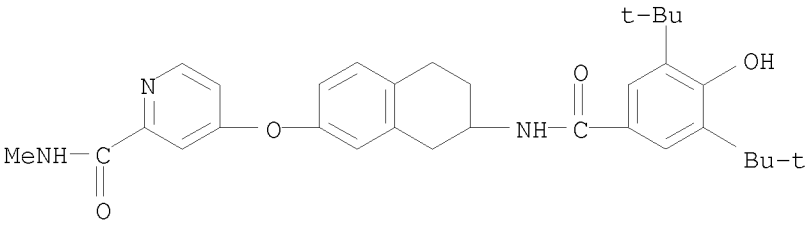
AB Bicyclic aryl compds. B-G1-A-G2-C {A = (un)substituted fused bicycle with at least one benzene ring such as 2,7-naphthalenediyl, 3,6-quinolinediyl, 3,6-isoquinolinediyl, 2,7-quinolinediyl, 2,7-quinazolinediyl, etc.; B = (un)substituted nitrogen-containing monocyclic heteroaryl ring or an (un)substituted pyridine- or pyrimidine-fused lactam; C = (un)substituted five- or six-membered aryl or heteroaryl ring containing 0-3 nitrogen atoms and 0-1 oxygen or sulfur atoms; G1 = (un)substituted CH2, C(:O), O, S, S(:O), SO2, or imino; G2 = (un)substituted C(:O)NH or NHC(:O) [if G2 is attached to a nitrogen atom of A, then G2 = (un)substituted C(:O)NH]; I} such as II are prepared as kinase inhibitors (particularly for Raf kinases) for the treatment of cancer. II is prepared in six steps (longest linear sequence) from 7-methoxy-1-tetralone and 4-chloro-2-pyridinecarbonitrile; II is separated into its enantiomers by chiral HPLC. Hydrolysis of tetrahydronaphthalenecarboxylate III, coupling of the naphthalenecarboxylic acid and 4-chloro-3-(trifluoromethyl)aniline, boron tribromide-mediated demethylation to yield a phenol, and O-arylation of the phenol with IV yields II. III is prepared in two steps by Claisen condensation of 7-methoxy-1-tetralone with di-Me carbonate followed by reduction of the ketone, while IV is prepared by cyclocondensation of 4-chloro-2-pyridinecarbonitrile with 1,2-ethanediamine. Ranges of IC50 values for the inhibition of B-Raf and C-Raf kinases and for the inhibition of Raf kinases in A375 cells by approx. 300 of the invention compds. are determined Pharmaceutical compns. of I with an appropriate carrier are claimed.

IT 942075-03-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen-containing heteroaryl-substituted aryl bicycles as inhibitors of kinases such as B-Raf and C-Raf kinases for treatment of cancer)

RN 942075-03-8 CAPLUS

CN 2-Pyridinecarboxamide, 4-[[7-[[3,5-bis(1,1-dimethylethyl)-4-

hydroxybenzoyl]amino]-5,6,7,8-tetrahydro-2-naphthalenyl]oxy]-N-methyl-
(CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:607873 CAPLUS
DOCUMENT NUMBER: 147:212376
TITLE: Synthesis of an optically active helical poly(1,3-phenyleneethynylene) bearing stable radicals and its chiroptical and magnetic properties
AUTHOR(S): Kaneko, Takashi; Yoshimoto, Shota; Hadano, Shingo; Teraguchi, Masahiro; Aoki, Toshiki
CORPORATE SOURCE: Center for Transdisciplinary Research, Niigata University, Niigata, 950-2181, Japan
SOURCE: Polyhedron (2007), 26(9-11), 1825-1829
CODEN: PLYHDE; ISSN: 0277-5387
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

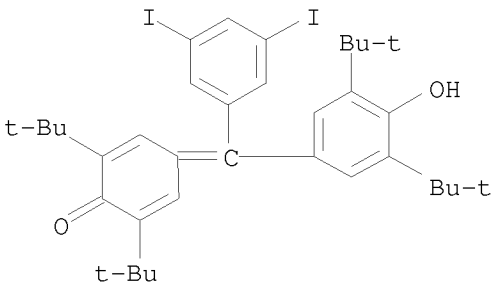
AB We synthesized an optically active helical poly(1,3-phenyleneethynylene) with pendant galvinoxyl residues and dimethyl(10-(1S)-pinanyl)silyl groups. The hydrogalvinoxyl precursor polymer was given by polymerization of (1,3-diiodophenyl)hydrogalvinoxyl and 1,3-diethynyl-5-[dimethyl(10-(1S)-pinanyl)silyl]benzene using Pd(PPh3)4 catalyst (Mw = 1.7 + 105, Mw/Mn = 3.7). In the CD spectrum taken in Et acetate solution, clear Cotton effects were observed in the absorption region of the backbone and hydrogalvinoxyl chromophore, indicating an excess of one-handed helical foldamer conformation. The polymer yielded the corresponding polyradical with high spin concentration by treatment of the polymer solution with PbO2. The Cotton effects appeared in CD spectra of the polymer and polyradical by addition of methanol to the chloroform solution, although the Cotton effects were hardly observed in chloroform. On the other hand, in the MCD spectra of the polymer and polyradical taken in chloroform solution, Faraday effects were observed in the absorption region of the backbone and galvinoxyl chromophore. The static magnetic susceptibility of the chiral polyradical was measured using a SQUID magnetometer, and showed the antiferromagnetic interaction.

IT 945263-39-8P 945263-40-1P 945263-42-3P
945263-44-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of optically active helical poly(phenyleneethynylene) bearing stable radicals and its chiroptical and magnetic properties)

RN 945263-39-8 CAPLUS
CN 2,5-Cyclohexadien-1-one, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl](3,5-diiodophenyl)methylene]-2,6-bis(1,1-dimethylethyl)-, polymer with (1S,5S)-2-[[(3,5-diethynylphenyl)dimethylsilyl]methyl]-6,6-dimethylbicyclo[3.1.1]heptane (CA INDEX NAME)

CM 1

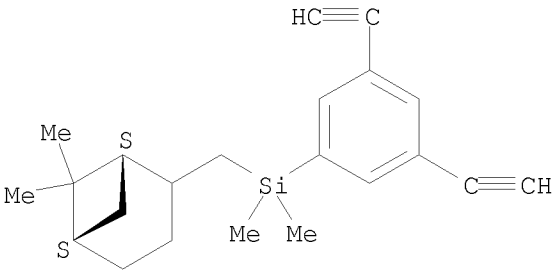
CRN 945263-38-7
CMF C35 H44 I2 O2



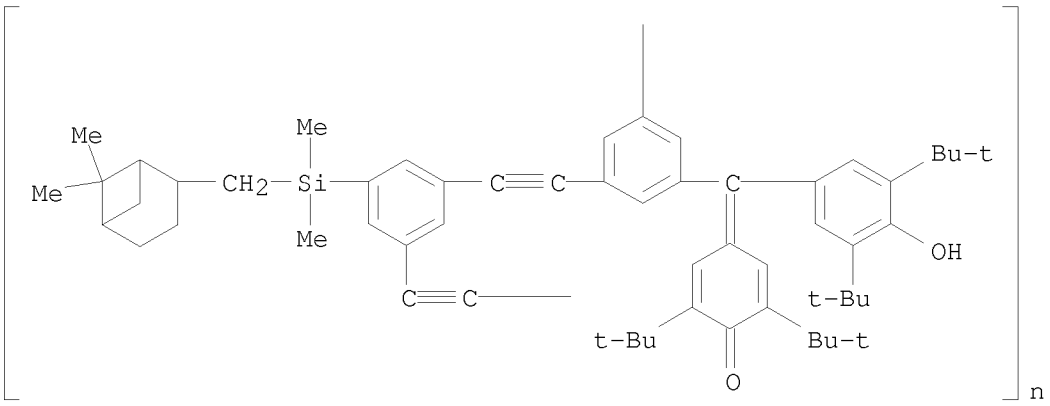
CM 2

CRN 945263-37-6
CMF C22 H28 Si

Absolute stereochemistry.



RN 945263-40-1 CAPLUS
CN Poly[[5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl][3,5-bis(1,1-dimethylethyl)-4-oxo-2,5-cyclohexadien-1-ylidene]methyl]-1,3-phenylene]-1,2-ethynedily[5-[[[(1S,5S)-6,6-dimethylbicyclo[3.1.1]hept-2-yl]methyl]dimethylsilyl]-1,3-phenylene]-1,2-ethynediyl] (CA INDEX NAME)



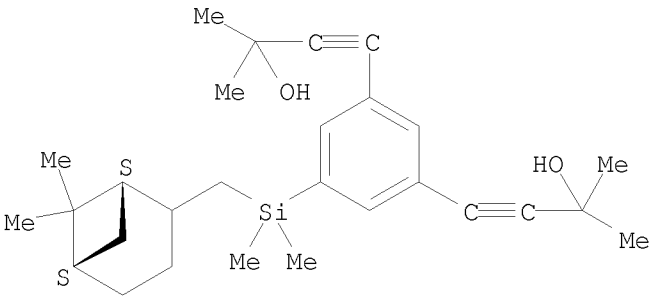
RN 945263-42-3 CAPLUS
CN 2,5-Cyclohexadien-1-one, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl](3,5-diiodophenyl)methylene]-2,6-bis(1,1-dimethylethyl)-,

polymer with (1S,5S)-2-[[[3,5-bis(3-hydroxy-3-methyl-1-butyn-1-yl)phenyl]dimethylsilyl]methyl]-6,6-dimethylbicyclo[3.1.1]heptane (CA INDEX NAME)

CM 1

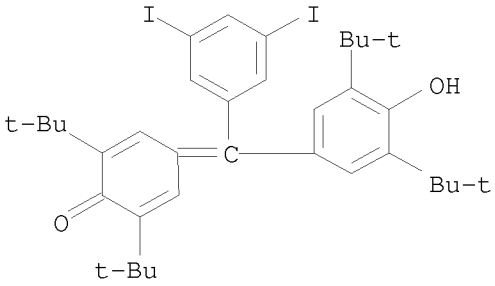
CRN 945263-41-2
CMF C28 H40 O2 Si

Absolute stereochemistry.



CM 2

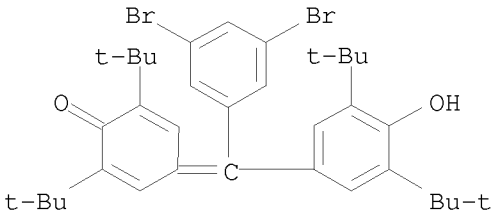
CRN 945263-38-7
CMF C35 H44 I2 O2



RN 945263-44-5 CAPLUS
CN 2,5-Cyclohexadien-1-one, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl](3,5-dibromophenyl)methylene]-2,6-bis(1,1-dimethylethyl)-, polymer with (1S,5S)-2-[[[3,5-bis(3-hydroxy-3-methyl-1-butyn-1-yl)phenyl]dimethylsilyl]methyl]-6,6-dimethylbicyclo[3.1.1]heptane (CA INDEX NAME)

CM 1

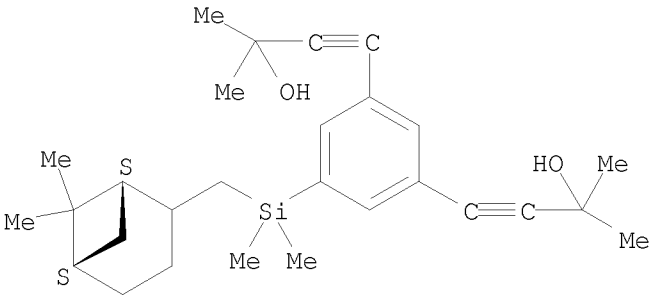
CRN 945263-43-4
CMF C35 H44 Br2 O2



CM 2

CRN 945263-41-2
CMF C28 H40 O2 Si

Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

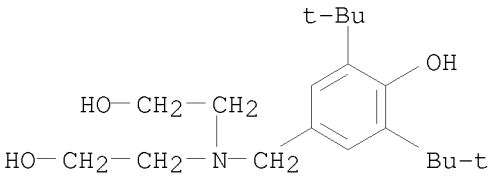
L5 ANSWER 5 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1331240 CAPLUS
DOCUMENT NUMBER: 146:220122
TITLE: QSAR study of anticoccidial activity for diverse chemical compounds: Prediction and experimental assay of trans-2-(2-nitrovinyl)furan
AUTHOR(S): Gonzalez-Diaz, Humberto; Olazabal, Ervelio; Santana, Lourdes; Uriarte, Eugenio; Gonzalez-Diaz, Yenny; Castanedo, Nilo
CORPORATE SOURCE: Department of Organic Chemistry & Institute of Industrial Pharmacy, Faculty of Pharmacy, University of Santiago de Compostela, Santiago, 15782, Spain
SOURCE: Bioorganic & Medicinal Chemistry (2007), 15(2), 962-968
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In this work the authors report a QSAR model that discriminates between chemical heterogeneous classes of anticoccidial and nonanticoccidial compds. For this purpose the authors used the Markovian Chems. in silico Design (MARCH-INSIDE) approach [Gonzalez-Diaz et al. J. Mol. Mod. 2002, 8, 237-245; J. Mol. Mod. 2003, 9, 395-407]. Linear discriminant anal. allowed us to fit the discriminant function. This function correctly classifies 86.67% of anticoccidial compds. and 96.23% of inactive compds. in the training series. Overall classification is 94.12%. The authors validated the model by means of an external predicting series, with 86.96% of global predictability. Remarkably, the present model is based on topol. as well as configuration-dependent mol. descriptors. Therefore,

the model performs timely calcns. and allows discrimination between Z/E and chiral isomers. Finally, to exemplify the use of the model in practice the authors report the prediction and exptl. assay of trans-2-(2-nitrovinyl)furan. It is notable that lesion control was 72.86% at mg/kg of body weight with respect to 60% at 125 mg/kg for amprolium (control drug). The back-projection map for this compound predicts a high level of importance for the double bond and for the nitro group in the trans position. The authors conclude that the MARCH-INSIDE approach enables the accurate fast track identification of anticoccidial hits. Moreover, trans-2-(2-nitrovinyl)furan seems to be a promising drug for the treatment of coccidiosis.

IT 2226-97-3, Ambunol
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR study of anticoccidial activity and identification of trans-2-(2-nitrovinyl)furan as coccidiostat)

RN 2226-97-3 CAPLUS

CN Phenol, 4-[[bis(2-hydroxyethyl)amino]methyl]-2,6-bis(1,1-dimethylethyl)-, hydrochloride (1:1) (CA INDEX NAME)



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:826307 CAPLUS
DOCUMENT NUMBER: 145:256434
TITLE: Discovery of a Solid Solution of Enantiomers in a Racemate-Forming System by Seeding
AUTHOR(S): Huang, Jun; Chen, Shuang; Guzei, Ilia A.; Yu, Lian
CORPORATE SOURCE: School of Pharmacy, University of Wisconsin- Madison, Madison, WI, 53705, USA
SOURCE: Journal of the American Chemical Society (2006), 128(36), 11985-11992
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

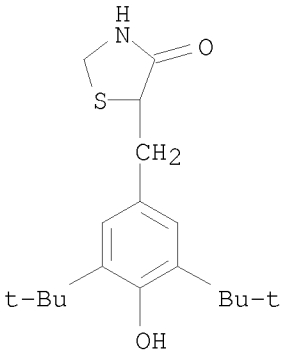
AB A racemic liquid of opposite enantiomers usually crystallizes as a racemic compound (racemate), rarely as a conglomerate, and even more rarely as a solid solution We discovered a Type II solid solution (mixed crystal) of the enantiomers of the chiral drug tazofelone (TZF) by seeding its racemic liquid with enantiomerically pure crystals (enantiomorphs). Without seeding, the racemic liquid crystallized as a racemic compound The crystal structure of this solid solution resembles that of the enantiomorph but has static disorder arising from the random substitution of enantiomers. This solid solution is a kinetic product of crystallization made possible by its faster growth rate compared to that of the competing racemate (by 4- to 40-fold between 80 and 146°). The free energy of the solid solution continuously varies with the enantiomeric composition between those of the

conglomerate and the racemates. The existence of the TZF solid solution explains the absence of eutectic melting between crystals of different enantiomeric compns. The ability of TZF to simultaneously form racemate and solid solution originates from its conformational flexibility. Similar solid solns. of enantiomers may exist in other systems and may be discovered in similar ways. The study demonstrates the use of cross-nucleation for discovering and engineering crystalline materials to optimize phys. properties.

IT 107902-67-0, Tazofelone
RL: ANT (Analyte); ANST (Analytical study)
(discovery of a solid solution of enantiomers in a racemate-forming system by seeding)

RN 107902-67-0 CAPLUS

CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]- (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:403577 CAPLUS
DOCUMENT NUMBER: 145:438759
TITLE: Method for preparing chiral spiro phosphites and their application in asymmetric addition
INVENTOR(S): Zhou, Qilin; Duan, Haifeng; Shi, Wenjian; Wang, Lixin; Xie, Jianhua
PATENT ASSIGNEE(S): Nankai University, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 16 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

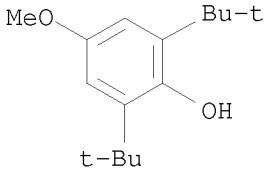
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1760198	A	20060419	CN 2005-10015985	20051109

PRIORITY APPLN. INFO.: CN 2005-10015985 20051109
OTHER SOURCE(S): CASREACT 145:438759; MARPAT 145:438759

AB The novel spiro compds. O,O'-[1,1'-spirobiindan-7,7'-diyl] O-alkyl-phosphite or O,O'-[1,1'-spirobiindan-7,7'-diyl] O-aryl-phosphite are prepared the reaction of 7,7'-dihydroxy-1,1'-spirobiindane with (i) phosphorus trichloride followed by treating with corresponding alc.; (ii) alkoxy/aryloxyphosphorus dichloride, or (iii) dimethylamine phosphite followed by treating with phenol or alc. to obtain the title compound The title compds. can be used in rhodium-complex catalysts for aldehyde asym. addition with aryl-boric acid or for imine asym. addition with aryl-boric acid.

IT 489-01-0

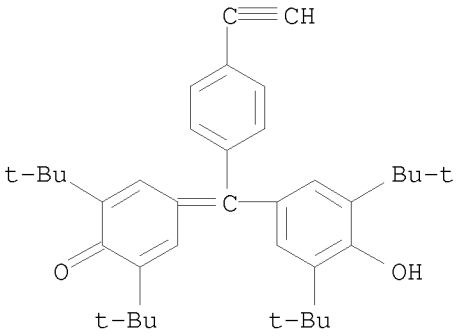
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chiral spiro phosphite ligands and the rhodium(I) complexes as catalysts for asym. addition reaction)
RN 489-01-0 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-methoxy- (CA INDEX NAME)



L5 ANSWER 8 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1107041 CAPLUS
DOCUMENT NUMBER: 144:36566
TITLE: Assignment of Helical Sense for Poly(phenylacetylene) Bearing Achiral Galvinoxyl Chromophore Synthesized by Helix-Sense-Selective Polymerization
AUTHOR(S): Kaneko, Takashi; Umeda, Yasuhiro; Yamamoto, Tsuyoshi; Teraguchi, Masahiro; Aoki, Toshiki
CORPORATE SOURCE: Department of Chemistry and Chemical Engineering, Faculty of Engineering and Graduate School of Science and Technology, and Center for Transdisciplinary Research, Niigata University, Niigata, 950-2181, Japan
SOURCE: Macromolecules (2005), 38(23), 9420-9426
CODEN: MAMOBX; ISSN: 0024-9297
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB {4-[(3,5-Di-tert-butyl-4-hydroxyphenyl)(3,5-di-tert-butyl-4-oxocyclohexa-2,5-dienylidene)methyl]phenyl}acetylene (abbreviated as (4-ethynylphenyl)hydrogalvinoxyl) was polymerized using [Rh(norbornadiene)Cl]2 catalyst in the presence of (R)-1-phenylethylamine or (S)-1-phenylethylamine to give red polymers. The CD (CD) spectra of polymers indicated that an excess of one-handed helical polyacetylene backbone was induced by helix-sense-selective polymerization under the asym. condition despite the achiral monomer. Results show that the CD signal intensity depends on temperature and decreases reversibly with increasing temperature, although the energy difference between the right-handed and left-handed conformations of each other is almost zero. The sign of the CD signal in the absorption region (420 nm) of the hydrogalvinoxyl chromophore, which was calculated from the polymer geometry, suggests that the excess of right-handed helix was induced by polymerization in the presence of (R)-1-phenylethylamine.
IT 129217-05-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(template; helix-sense-selective polymerization of (ethynylphenyl)hydrogalvinoxyl in the presence of chiral phenylethylamines)
RN 129217-05-6 CAPLUS
CN 2,5-Cyclohexadien-1-one, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl](4-ethynylphenyl)methylene]-2,6-bis(1,1-dimethylethyl)-, homopolymer (CA INDEX NAME)

CM 1

CRN 129216-99-5
CMF C37 H46 O2

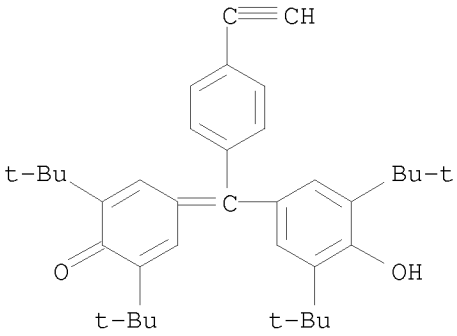


REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:548882 CAPLUS
DOCUMENT NUMBER: 143:194350
TITLE: Helix-sense-selective polymerization of a phenylacetylene bearing an achiral and bulky galvinoxyl moiety
AUTHOR(S): Umeda, Yasuhiro; Kaneko, Takashi; Teraguchi, Masahiro; Aoki, Toshiki
CORPORATE SOURCE: Department of Chemistry and Chemical Engineering, Faculty of Engineering, Niigata University, Niigata, 950-2181, Japan
SOURCE: Chemistry Letters (2005), 34(6), 854-855
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An achiral and bulky phenylacetylene monomer, (4-ethynylphenyl)hydrogalvinoxyl, was polymerized using [Rh(nbd)Cl]2 (nbd = 2,5-norbornadiene) catalyst in chiral phenylethylamine. The CD spectra of the obtained polymers indicated that an excess of one-handed helical polyacetylene backbone was induced by helix-sense-selective polymerization despite the achiral monomer.
IT 129217-05-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(helix-sense-selective polymerization of a phenylacetylene bearing an achiral
and bulky galvinoxyl moiety in the presence of chiral phenylethylamine)
RN 129217-05-6 CAPLUS
CN 2,5-Cyclohexadien-1-one, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl](4-ethynylphenyl)methylene]-2,6-bis(1,1-dimethylethyl)-, homopolymer (CA INDEX NAME)

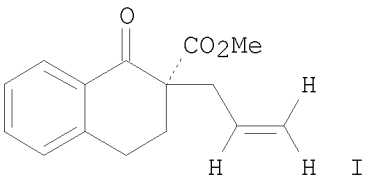
CM 1

CRN 129216-99-5
CMF C37 H46 O2



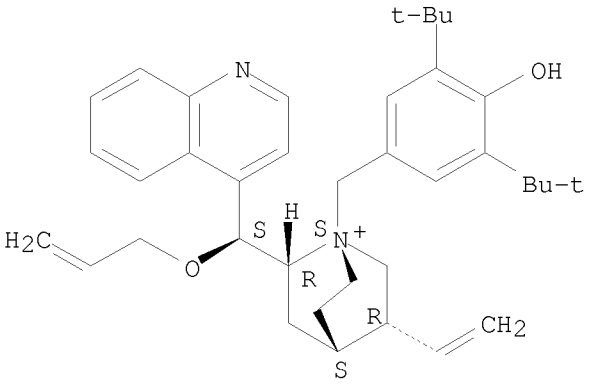
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:725588 CAPLUS
DOCUMENT NUMBER: 141:365973
TITLE: Enantioselective alkylation of β-keto esters by phase-transfer catalysis using chiral quaternary ammonium salts
AUTHOR(S): Park, Eun Joo; Kim, Mi Hee; Kim, Dae Young
CORPORATE SOURCE: Department of Chemistry, Soonchunhyang University, Chungnam, 336-600, S. Korea
SOURCE: Journal of Organic Chemistry (2004), 69(20), 6897-6899
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:365973
GI



AB A catalytic enantioselective alkylation procedure, promoted by a quaternary ammonium salt from cinchonine as a phase transfer catalyst, is described. Treatment of cyclo β-keto esters with alkyl halide under mild reaction conditions afforded α-alkylated β-keto esters, e.g., I, in moderate to excellent yields with high enantiomeric excesses.
IT 405506-36-7 405506-37-8
RL: CAT (Catalyst use); USES (Uses)
(stereoselective preparation of α-alkyl-β-keto ester via asym. alkylation of β-keto esters with alkyl halides or butenone under phase-transfer catalysis using chiral quaternary ammonium salts as catalyst)
RN 405506-36-7 CAPLUS
CN Cinchonanium, 1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-9-(2-propenyloxy)-, bromide, (9S)- (9CI) (CA INDEX NAME)

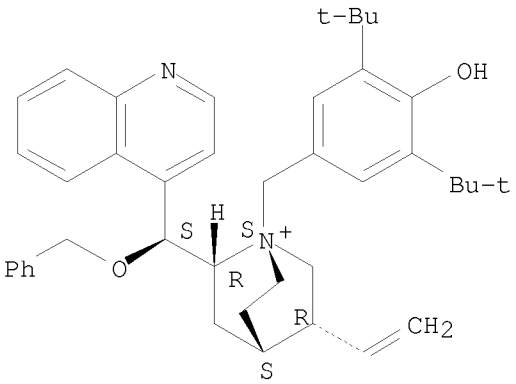
Absolute stereochemistry.



● Br^-

RN 405506-37-8 CAPLUS
CN Cinchonanium, 1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-9-(phenylmethoxy)-, bromide, (9S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

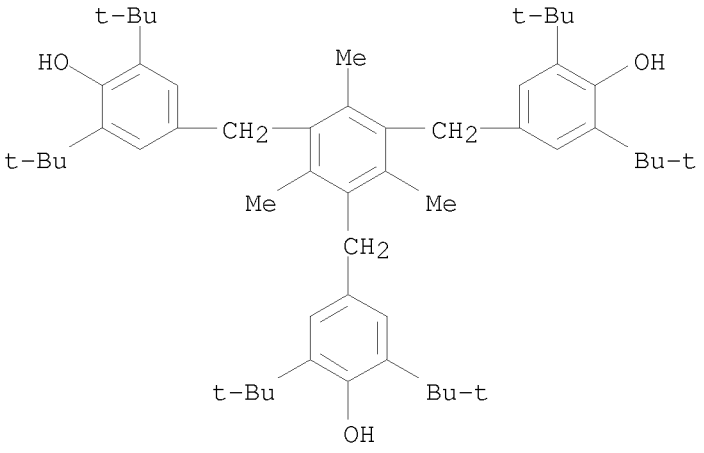
L5 ANSWER 11 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:571924 CAPLUS
DOCUMENT NUMBER: 139:261226
TITLE: Enhancement of the efficiency of the low temperature method for kinetic resolution of primary alcohols by optimizing the organic bridges in porous ceramic-immobilized lipase
AUTHOR(S): Sakai, Takashi; Hayashi, Kyoko; Yano, Fumika; Takami, Mie; Ino, Megumi; Korenaga, Toshinobu; Ema, Tadashi
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Okayama University, Okayama, 700-8530, Japan
SOURCE: Bulletin of the Chemical Society of Japan (2003), 76(7), 1441-1446

CODEN: BCSJA8; ISSN: 0009-2673
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:261226

AB For the enhancement of enantioselectivity and acceleration of the reaction rate in the lipase-catalyzed resolution of primary alcs., the use of a very low reaction temperature (-30 °C) and an immobilized lipase on organic bridges-coated porous ceramic support was found to be highly effective. Furthermore, the structure of the organic bridges greatly influenced the temperature effect between ln E and 1/T as well as the reaction rate. Among the organic bridges examined in the resolution of (±)-2-hydroxymethyl-1,4-benzodioxane, the 6-(2-methylpropanoyloxy)hexylsilanetrioxyl bridge was the best choice for both the E value and the reaction rate at -30 °C. Lipase was immobilized in toyonite 200 modified with 2-methyl-2-propenoic acid 3-(trimethoxysilyl)propyl ester, 2-methyl-2-propenoic acid 6-(trimethoxysilyl)hexyl ester, 2-methyl-2-propenoic acid 6-(trimethoxysilyl)undecyl ester, 2-methylpropanoic acid 6-(trimethoxysilyl)undecyl ester, 6-(trimethoxysilyl)-1-hexanol acetate, etc. Toyonite-immobilized lipases were used for the resolution of β-methylbenzeneethanol which gave (βS)-β-methylbenzeneethanol acetate and (βR)-β-methylbenzeneethanol.

IT 1709-70-2
RL: RGT (Reagent); RACT (Reactant or reagent)
(enhancement of efficiency of low temperature method for kinetic resolution of primary alcs. by optimizing organic bridges in porous ceramic-immobilized lipase)

RN 1709-70-2 CAPLUS
CN Phenol, 4,4',4''-[(2,4,6-trimethyl-1,3,5-benzenetriyl)tris(methylene)]tris[2,6-bis(1,1-dimethylethyl)- (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 12 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:319885 CAPLUS
DOCUMENT NUMBER: 138:338158
TITLE: Preparation of benzoxazine- and benzothiazine-containing

β-aryl-α-oxypropionic acid derivatives and pharmaceutical compositions containing them as hPPARα and hPPARγ agonists with therapeutic uses

INVENTOR(S): Bhuniya, Debnath; Das, Saibal Kumar; Madhavan, Gurram Ranga; Iqbal, Javed; Chakrabarti, Ranjan

PATENT ASSIGNEE(S): Reddy's Laboratories Ltd., India

SOURCE: PCT Int. Appl., 161 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

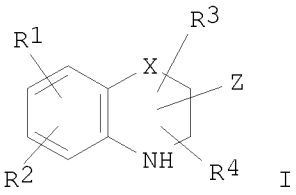
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003033481	A1	20030424	WO 2002-IB4275	20021015
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
IN 2001MA00848	A	20050304	IN 2001-MA848	20011016
CA 2463686	A1	20030424	CA 2002-2463686	20021015
AU 2002341289	A1	20030428	AU 2002-341289	20021015
AU 2002341289	B2	20080724		
EP 1436268	A1	20040714	EP 2002-775090	20021015
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002013350	A	20041013	BR 2002-13350	20021015
HU 2004001649	A2	20041129	HU 2004-1649	20021015
HU 2004001649	A3	20070529		
CN 1589258	A	20050302	CN 2002-822723	20021015
CN 1596249	A	20050316	CN 2002-823822	20021015
JP 2005527480	T	20050915	JP 2003-536221	20021015
NZ 532284	A	20060224	NZ 2002-532284	20021015
CN 1982299	A	20070620	CN 2006-10156228	20021015
ZA 2004002858	A	20050112	ZA 2004-2858	20040415
MX 2004PA03628	A	20040730	MX 2004-PA3628	20040416
ZA 2004002910	A	20050113	ZA 2004-2910	20040416
NO 2004001998	A	20040702	NO 2004-1998	20040514
US 20050113368	A1	20050526	US 2004-492454	20041217
US 7365064	B2	20080429		

PRIORITY APPLN. INFO.:

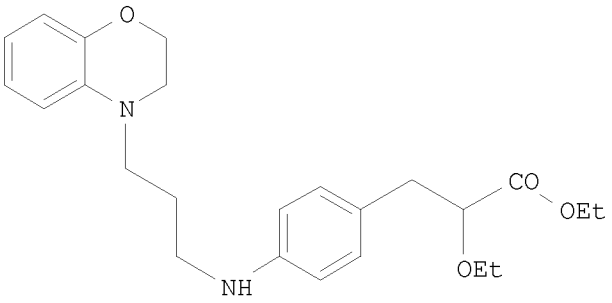
IN 2001-MA848	A	20011016
IN 2001-CH848	A	20011016
CN 2002-823822	A3	20021015
WO 2002-IB4275	W	20021015

OTHER SOURCE(S): MARPAT 138:338158

GI



I



II

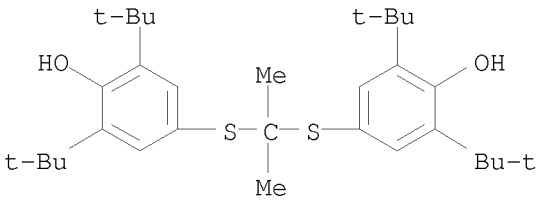
AB The present invention relates to novel antidiabetic, hypolipidemic, antiobesity and hypocholesterolemic benzoxazine and benzothiazine derivs. (shown as I; variables defined below; e.g. Et 3-[4-[[3-(3,4-dihydro-2H-benzo[b][1,4]oxazin-4-yl)propyl]amino]phenyl]-2-ethoxypropanoate (II)), their analogs, their tautomeric forms, their stereoisomers, their polymorphs, their pharmaceutically acceptable salts, their pharmaceutically acceptable solvates and pharmaceutically acceptable compns. containing them, to a process for preparing such compds. and intermediates involved in preparation of I. Several methods of preparation are claimed and 22 example prepns. of intermediates and 72 of I are included. For example, II was prepared in 30% yield from Et 2-ethoxy-3-(4-aminophenyl)propanoate, 3-(3,4-dihydro-2H-benzo[b][1,4]oxazin-4-yl)propyl bromide and K2CO3 in DMF. The reactant Et 2-ethoxy-3-(4-aminophenyl)propanoate was prepared in 60 % yield from the Wittig salt, from tri-Et 2-ethoxyphosphonoacetate and NaH, and 4-nitrobenzaldehyde followed by hydrogenation. The other reactant, 3-(3,4-dihydro-2H-benzo[b][1,4]oxazin-4-yl)propyl bromide, was obtained in 47% yield from 3,4-dihydro-2H-benzo[b][1,4]oxazine, 1,3-dibromopropane and Na2CO3 in DMF. The efficacy of I was demonstrated via the following tests: in vitro hPPARα and hPPARγ activities and in vivo reduction in blood glucose and triglyceride, total cholesterol, LDL and VLDL levels and increase in HDL level. For I: R1, R2 and R3, R4 when attached to C = H, halogen, hydroxy, nitro, cyano, formyl or (un)substituted alkyl, cycloalkyl, alkoxy, cycloalkoxy, aryl, aryloxy, aralkyl, aralkoxy, heterocyclyl, heteroaryl, heteroaralkyl, heteroaryloxy, heteroaralkoxy, acyl, acyloxy, hydroxyalkyl, amino, acylamino, monoalkylamino, dialkylamino, arylamino, aralkylamino, alkoxycarbonyl, aryloxycarbonyl, aralkoxycarbonyl, alkoxyalkyl, aryloxyalkyl, aralkoxyalkyl, alkylthio, thioalkyl, alkoxycarbonylamino, aryloxycarbonylamino, aralkoxycarbonylamino, carboxylic acid or its derivs., or sulfonic acid or its derivs.; one or both of R3 and R4 = oxo or thioxo group when they are attached to C. R3 and R4 when attached to N = H, hydroxy, formyl or (un)substituted alkyl, cycloalkyl, alkoxy, cycloalkoxy, aryl, aralkyl, heterocyclyl, heteroaryl, heteroaralkyl, acyl, acyloxy, hydroxyalkyl, amino, acylamino, monoalkylamino, dialkylamino, arylamino, aralkylamino, aminoalkyl, aryloxy, aralkoxy, heteroaryloxy, heteroaralkoxy, alkoxycarbonyl, aryloxycarbonyl, aralkoxycarbonyl, alkoxyalkyl, aryloxyalkyl, aralkoxyalkyl, alkylthio, thioalkyl groups, carboxylic acid derivs., or sulfonic acid derivs. X = O or S; Z = (CR10R11)n-W-(CR10R11)m-Ar-CHR5CR6(OR7)C(O)YR8; W = NR12, -C(O)(CR10R11)oNR12, -O-aryl-(CR10R11)o-NR12, where R12 = H or (un)substituted alkyl, aryl or aralkyl; o = 0-6; R10 and R11 = H or

(un)substituted alkyl, alkoxy, aryl or aralkyl; Ar = (un)substituted divalent single or fused aromatic or heterocyclic divalent phenylene, naphthylene, pyrrolyl, pyridyl, quinolinyl, benzofuryl, dihydrobenzofuryl, benzopyranyl, dihydrobenzopyranyl, indolyl, indolinyl, azaindolyl, azaindolinyl, pyrazolyl, benzothiazolyl or benzoxazolyl; R5 = H, hydroxy, alkoxy, halogen, alkyl, (un)substituted aralkyl or forms a bond together with the adjacent group R6. R6 = H, hydroxy, alkoxy, halogen, alkyl, acyl, (un)substituted aralkyl or R6 forms a bond together with R5; R7 = H or (un)substituted alkyl, cycloalkyl, aryl, aralkyl, alkoxyalkyl, alkoxycarbonyl, aryloxycarbonyl, alkylaminocarbonyl, arylaminocarbonyl, acyl, heterocyclyl, heteroaryl, heteroaralkyl; R8 = H or (un)substituted alkyl, cycloalkyl, aryl, aralkyl, heterocyclyl, heteroaryl or heteroaralkyl; Y = O, S or NR9, where R9 = H or (un)substituted alkyl, aryl, hydroxyalkyl, aralkyl heterocyclyl, heteroaryl, or heteroaralkyl or NR9 = chiral amine, chiral amine alcs. derived from chiral amino acid; or R8 and R9 together form a (un)substituted 5 or 6 membered cyclic structure containing C atoms, which optionally contain ≥1 heteroatoms = O, S or N; m and n = 0-6.

IT 23288-49-5, Probucol
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combined with benzoxazine- and benzothiazine-containing β-aryl-α-oxypropionic acid derivative as hPPARα and hPPARγ agonists with therapeutic uses)

RN 23288-49-5 CAPLUS

CN Phenol, 4,4'-[(1-methylethylidene)bis(thio)]bis[2,6-bis(1,1-dimethylethyl)- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:93720 CAPLUS

DOCUMENT NUMBER: 138:321040

TITLE: Synthesis, Resolution, and Absolute Stereochemistry of (-)-Blestriarene C

AUTHOR(S): Hattori, Tetsutaro; Shimazumi, Yuhi; Goto, Hitoshi; Yamabe, Osamu; Morohashi, Naoya; Kawai, Wataru; Miyano, Sotaro

CORPORATE SOURCE: Department of Biomolecular Engineering, Graduate School of Engineering, Tohoku University, Sendai, 980-8579, Japan

SOURCE: Journal of Organic Chemistry (2003), 68(6), 2099-2108
CODEN: JOCEAH; ISSN: 0022-3263

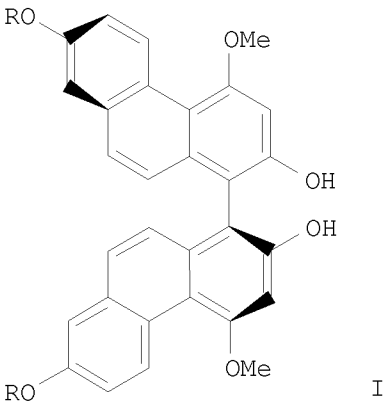
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:321040

GI



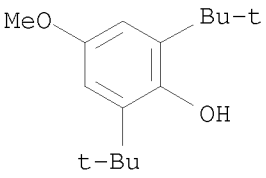
I

AB A naturally occurring 1,1'-biphenanthrene, blestriarene C (I; R = H), was prepared in 13 steps and 30% overall yield. The key steps are the ester-mediated nucleophilic aromatic substitution on 2,6-di-tert-butyl-4-methoxyphenyl 5-isopropoxy-2-methoxybenzoate by 2-methoxy-4-methoxymethoxy-6-methylphenylmagnesium bromide and a novel intramol. cyclization of the resulting 4-isopropoxy-2'-methoxy-4'-methoxymethoxy-6'-methylbiphenyl-2-carboxylic ester to 7-isopropoxy-4-methoxy-2-(methoxymethoxy)phenanthren-9-ol. The racemic blestriarene C was optically resolved by chiral HPLC on a preparative scale to give several 10-mg yields of both the enantiomers in up to 95% ee. The absolute stereochem. was determined to be Sa-(-) by the axial chirality recognition method, which was based on the stereospecific formation of a 12-membered cyclic diester containing two biaryl-o,o'-diyl unites joined by ester -CO2- linkages. The validity of the method was confirmed by an X-ray crystallog. anal. and ab initio conformational analyses of such 12-membered cyclic diesters. It was found that blestriarene C and its 7,7'-diisopropyl ether I (R = i-Pr) underwent rapid photoracemization even under ambient light exposure.

IT 489-01-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, resolution, and absolute stereochem. of (-)-blestriarene C)

RN 489-01-0 CAPLUS

CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-methoxy- (CA INDEX NAME)



REFERENCE COUNT: 107 THERE ARE 107 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:620040 CAPLUS

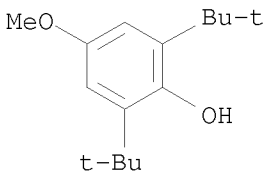
DOCUMENT NUMBER: 138:106235

TITLE: A chiral ligand-mediated asymmetric addition of a lithium BHA ester enolate to an aldehyde

AUTHOR(S): Nomura, Yumiko; Iguchi, Mayu; Doi, Hirohisa; Tomioka, Kiyoshi

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, The University of

Tokyo, Tokyo, 113-0033, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(8), 1131-1134
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:106235
AB The asym. reaction of a lithium enolate generated from a BHA, i.e., propanoic acid 2,6-bis(1,1-dimethylethyl)-4-methoxyphenyl ester, was allowed to react with benzaldehyde in the presence of a diether-type chiral ligand affording the corresponding anti-aldol product in a moderate enantioselectivity. A tetradentate ligand induced better enantioselectivity albeit relative loss of anti-selectivity. A variation of lithiating amide agent affected the selectivity, indicating involvement of an amine as a component of the mixed aggregate. Absolute configuration of some of the aldol products was determined by standard transformations.
IT 489-01-0, 2,6-Bis(1,1-dimethylethyl)-4-methoxyphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral dialkyl ether-type ligand-mediated asym. aldol addition of lithium propanoic acid 2,6-bis(1,1-dimethylethyl)-4-methoxyphenyl ester to aldehydes)
RN 489-01-0 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-methoxy- (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 15 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:386389 CAPLUS
DOCUMENT NUMBER: 137:125449
TITLE: Helical chirality of π-conjugated main-chain induced by polymerization of phenylacetylene with chiral bulky pinanyl groups: effects of the flexible spacer and polymerization catalyst
AUTHOR(S): Shinohara, Ken-Ichi; Aoki, Toshiki; Kaneko, Takashi
CORPORATE SOURCE: Center for Interdisciplinary Research (CIR), Department of Metallurgy, Graduate School of Engineering, Tohoku University, Sendai, 980-8578, Japan
SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry (2002), 40(11), 1689-1697
CODEN: JPACEC; ISSN: 0887-624X
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three optically active phenylacetylene polymers with chiral bulky pinanyl groups, (-)-poly[4-(dimethylpinanylsilyl)phenylacetylene] [(-)-poly(PSPA)], (+)-poly{4-[3-(10-pinanyl)tetramethyldisiloxy]phenylacethylene} [(+)-poly(PDSPA)], and their copolymer [(-)-copoly(PSPA/PDSPA)], were synthesized. We observed high chirality in the main-chain chromophore of (-)-poly(PSPA), due to the presence of a chiral helix, with CD spectroscopy. In contrast, (+)-poly(PDSPA), with flexible SiOSi spacers between the chiral

pinanyl group and the main chain, had lower chirality. (-)-Poly(PSPA), with large CD signals, was prepared by polymerization with a rhodium catalyst and had a highly stereoregular main chain (high cis-configuration percentage). However, (-)-poly(PSPA) prepared with a tungsten catalyst had lower chirality and lower stereoregularity in the main chain. A membrane from (-)-poly(PSPA) showed enantioselective permeability for tryptophan in an aqueous solution

IT 243662-26-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(optical rotation (-), high chirality; effects of the flexible spacer and polymerization catalyst on helical chirality of π-conjugated main-chain induced by polymerization of pinanyl-containing phenylacetylenes)

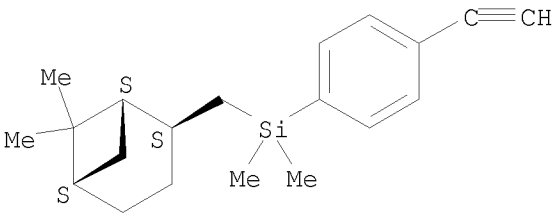
RN 243662-26-2 CAPLUS

CN 2,5-Cyclohexadien-1-one, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl](4-ethynylphenyl)methylene]-2,6-bis(1,1-dimethylethyl)-, polymer with [[(1S,2S,5S)-6,6-dimethylbicyclo[3.1.1]hept-2-yl]methyl](4-ethynylphenyl)dimethylsilane (9CI) (CA INDEX NAME)

CM 1

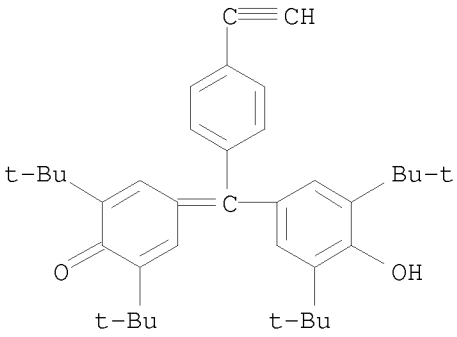
CRN 243662-25-1
CMF C20 H28 Si

Absolute stereochemistry. Rotation (-).



CM 2

CRN 129216-99-5
CMF C37 H46 O2



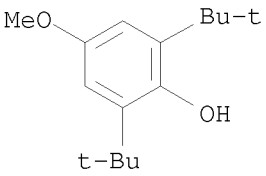
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:284195 CAPLUS
DOCUMENT NUMBER: 137:185085

TITLE: Conjugate addition of lithiated (s)-4-isopropyl-3-[(methylthio)methyl]-5,5-diphenyl-2-oxazolidinone to cinnamoyl derivatives: Preparation of enantiomerically pure 1,4-diols
AUTHOR(S): Gaul, Christoph; Seebach, Dieter
CORPORATE SOURCE: Laboratorium fur Organische Chemie der Eidgenossischen Technischen Hochschule, ETH-Honggerberg, Zurich, CH-8093, Switz.
SOURCE: Helvetica Chimica Acta (2002), 85(3), 772-787
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:185085

AB The Li derivative of (S)-4-isopropyl-3-[(methylthio)methyl]-5,5-diphenyl-2-oxazolidinone (synthetic equivalent to a chiral formyl anion) adds to enones and enoates in a 1,4-fashion. Best results are obtained with 1,3-diarylpropenones (chalcones), trityl enones, and 2,6-di(tert-butyl)-4-methoxyphenyl cinnamates, with yields up to 80% and diastereoselectivities up to and above 99:1 of the products containing three stereogenic centers. X-Ray crystal-structure anal. reveals that the C,C-bond formation occurs preferentially with relative topicity ul (Re/Si). The MeS group of the 1,4-adducts can be replaced by RO groups in Hg2+-assisted substitutions, with subsequent removal and facile recovery of the chiral auxiliary. 4-Hydroxycarbonyl derivs. (homoaldols) and mono-, di-, and trisubstituted 1,4-diols are, thus, accessible in enantiomerically pure forms.

IT 125995-56-4, Lithium 2,6-di(tert-butyl)-4-methoxyphenoxide
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn of enantiomerically pure 1,4-diols via diastereoselective conjugate addition of lithium (4S)-4-(1-methylethyl)-3-[(methylthio)methyl]-5,5-diphenyl-2-oxazolidinone (synthetic formyl anion equivalent) to cinnamoyl derivs.)
RN 125995-56-4 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-methoxy-, lithium salt (1:1) (CA INDEX NAME)

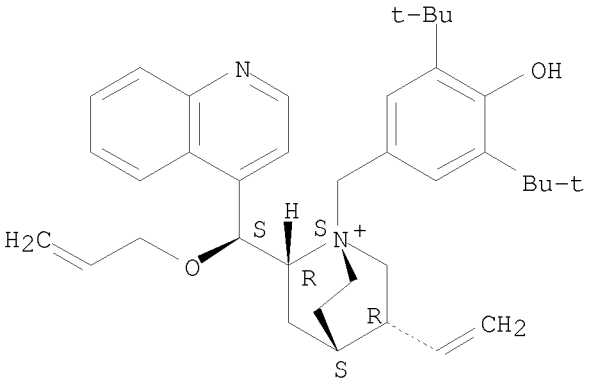


REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:73573 CAPLUS
DOCUMENT NUMBER: 136:279183
TITLE: Catalytic Enantioselective Fluorination of β-Keto Esters by Phase-Transfer Catalysis Using Chiral Quaternary Ammonium Salts
AUTHOR(S): Kim, Dae Young; Park, Eun Joo
CORPORATE SOURCE: Department of Chemistry, Soonchunhyang University, Chungnam, 336-600, S. Korea
SOURCE: Organic Letters (2002), 4(4), 545-547

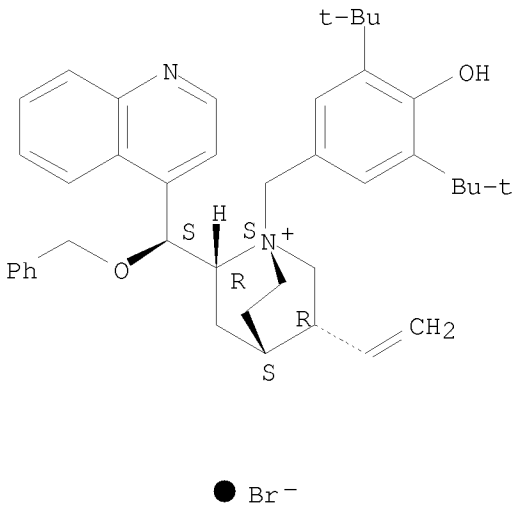
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:279183
AB The catalytic enantioselective electrophilic fluorination promoted by a quaternary ammonium salt from cinchonine as phase-transfer catalyst is described. Treatment of β-keto esters with N-fluorobenzenesulfonimide as the fluorine source under mild conditions afforded the α-fluoro β-keto esters in excellent yields with good to moderate enantiomeric excesses.
IT 405506-36-7 405506-37-8
RL: CAT (Catalyst use); USES (Uses)
(asym. fluorination of β-keto esters by phase-transfer catalysis using chiral quaternary ammonium salts)
RN 405506-36-7 CAPLUS
CN Cinchonanium, 1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-9-(2-propenyloxy)-, bromide, (9S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 405506-37-8 CAPLUS
CN Cinchonanium, 1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-9-(phenylmethoxy)-, bromide, (9S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 18 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:731406 CAPLUS
DOCUMENT NUMBER: 135:249524
TITLE: Process of preparing a reflective film
INVENTOR(S): Marden, Shirley Ann; Slaney, Kim; Verrall, Mark Andrew
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: Brit. UK Pat. Appl., 60 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

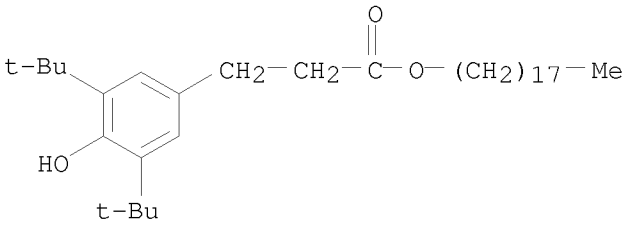
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2357291	A	20010620	GB 2000-29376	20001201
GB 2357291	B	20040317		

PRIORITY APPLN. INFO.: EP 1999-124834 A 19991214

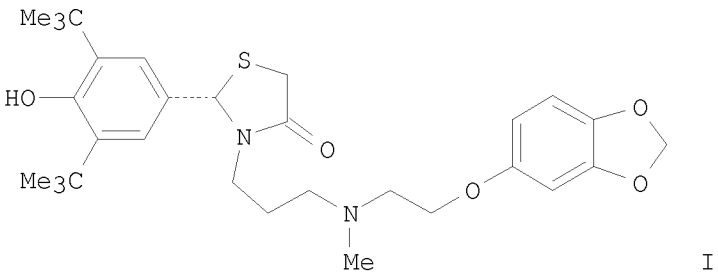
AB The invention relates to a process of preparing a reflective film comprising a layer of a polymerized mesogenic material with helically twisted structure, wherein the helix axis is perpendicular to the film plane, and containing regions with varying helical pitch. The invention relates to a polymerizable mesogenic material suitable for said process, to a reflective film obtainable by said process, to the use of such a reflective film as reflective broadband or notch polarizer or as a multicolored film or image in liquid crystal displays, as color filter, in effect pigments, for decorative or security applications, and to a liquid crystal display comprising a liquid crystal cell and a reflective polarizer as described in the foregoing and the following, and optionally further comprising one or more compensators or polarizers.

IT 2082-79-3, Irganox 1076
RL: CAT (Catalyst use); USES (Uses)
(preparation of helically twisted polymerized mesogenic reflective film containing)

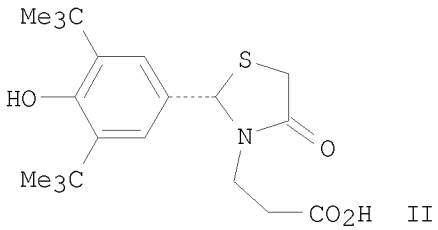
RN 2082-79-3 CAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (CA INDEX NAME)



L5 ANSWER 19 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:854602 CAPLUS
DOCUMENT NUMBER: 134:162959
TITLE: Practical synthesis of novel cardioprotective drug, CP-060S
AUTHOR(S): Kato, Tatsuya; Ozaki, Tomokazu; Tsuzuki, Kouichi; Ohi, Nobuhiro
CORPORATE SOURCE: Fuji Gotemba Research Laboratories, Chugai Pharmaceutical Company Ltd., Shizuoka, 412-8513, Japan
SOURCE: Organic Process Research & Development (2001), 5(2), 122-126
CODEN: OPRDFK; ISSN: 1083-6160
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:162959
GI



I

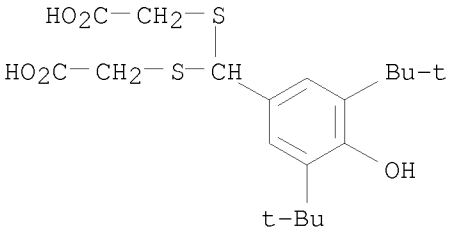


II

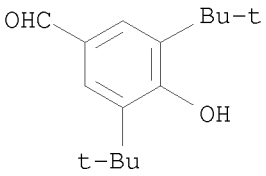
AB A practical synthesis of a novel cardioprotective drug, CP-060S (I), is described. Key intermediate (S)-(hydroxyphenyl)thiazolidinone II, a chiral carboxylic acid, was prepared from 3,5-di-tert-butyl-4-hydroxybenzaldehyde by employing thiazolidinone cyclocondensation followed by selective crystallization from a diastereomeric salt mixture which was prepared by treating racemic II with (S)-(-)-N-benzyl-α-methylbenzylamine (III). Racemization of the (R)-II-rich mixture, obtained from the mother liquid, by treatment with NaOH solution and subsequent resolution gave a second crop of (S)-II. Resolving agent III was efficiently recovered from the resolution process and pure

enough for recycling use. Chiral acid (S)-II was converted to the corresponding Me ester, which was reduced with NaBH4-CaCl2 to give alc. intermediate. Subsequent mesylation, amination, and salt formation with fumaric acid afforded CP-060S as pure enantiomer (99.8% ee) without any column chromatog.

IT 325172-06-3P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of cardioprotective thiazolidinone CP-060S)
RN 325172-06-3 CAPLUS
CN Acetic acid, 2,2'-[[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]bis(thio)]bis- (CA INDEX NAME)



IT 1620-98-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cardioprotective thiazolidinone CP-060S)
RN 1620-98-0 CAPLUS
CN Benzaldehyde, 3,5-bis(1,1-dimethylethyl)-4-hydroxy- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

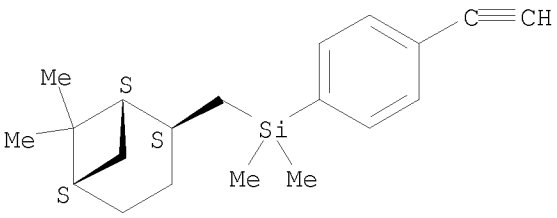
L5 ANSWER 20 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:446804 CAPLUS
DOCUMENT NUMBER: 131:214622
TITLE: Synthesis of an optically active poly(phenylacetylene) bearing galvinoxyl radicals for magnetic materials
AUTHOR(S): Kaneko, Takashi; Yamamoto, Tsuyoshi; Aoki, Toshiki; Oikawa, Eizo
CORPORATE SOURCE: Department of Chemistry and Chemical Engineering, Faculty of Engineering, Niigata University, Niigata, 950-2181, Japan
SOURCE: Chemistry Letters (1999), (7), 623-624
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An optically active polyradical was first synthesized by copolymn. of (4-ethynylphenyl)hydrogalvinoxyl and chiral acetylene monomer using Rh-catalyst. The CD spectrum of the polyradical showed a Cotton effect indicating the excess of one-handed helix backbone and the induced chirality of side-chain galvinoxyl units. Intermol. antiferromagnetic interaction observed for the polyradical was larger than that of the corresponding polyradical without excess of one-handed helix.

IT 243662-26-2DP, polyradical 243662-26-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of an optically active poly(phenylacetylene) bearing galvinoxyl radicals for magnetic materials)
RN 243662-26-2 CAPLUS
CN 2,5-Cyclohexadien-1-one, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl](4-ethynylphenyl)methylene]-2,6-bis(1,1-dimethylethyl)-, polymer with [[(1S,2S,5S)-6,6-dimethylbicyclo[3.1.1]hept-2-yl]methyl](4-ethynylphenyl)dimethylsilane (9CI) (CA INDEX NAME)

CM 1

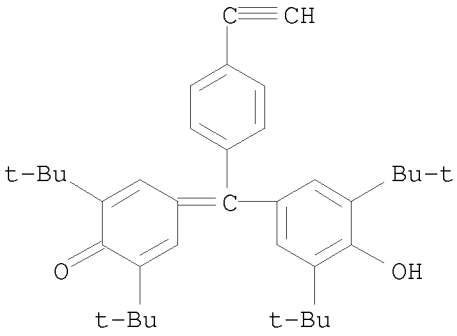
CRN 243662-25-1
CMF C20 H28 Si

Absolute stereochemistry. Rotation (-).



CM 2

CRN 129216-99-5
CMF C37 H46 O2

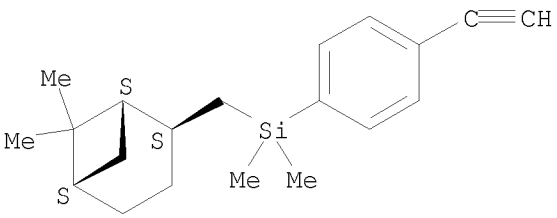


RN 243662-26-2 CAPLUS
CN 2,5-Cyclohexadien-1-one, 4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl](4-ethynylphenyl)methylene]-2,6-bis(1,1-dimethylethyl)-, polymer with [[(1S,2S,5S)-6,6-dimethylbicyclo[3.1.1]hept-2-yl]methyl](4-ethynylphenyl)dimethylsilane (9CI) (CA INDEX NAME)

CM 1

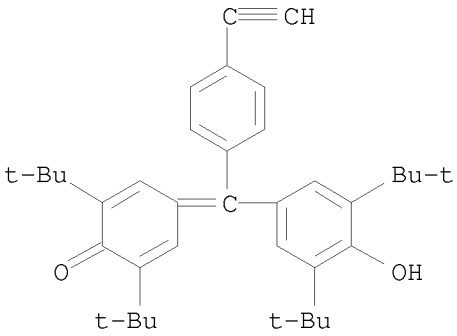
CRN 243662-25-1
CMF C20 H28 Si

Absolute stereochemistry. Rotation (-).



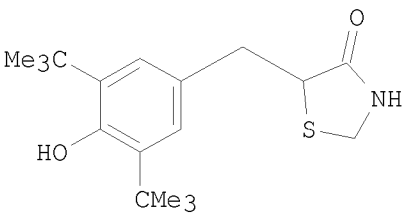
CM 2

CRN 129216-99-5
CMF C37 H46 O2



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 21 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:493672 CAPLUS
DOCUMENT NUMBER: 127:190676
ORIGINAL REFERENCE NO.: 127:36981a,36984a
TITLE: Substrate specificity of the kinetic resolution of sulfides by enantioselective sulfoxide formation
AUTHOR(S): Phillips, Michael L.; Panetta, Jill A.
CORPORATE SOURCE: Lilly Research Laboratories, Eli Lilly and Company, Lilly Corporate Center, Indianapolis, IN, 46285, USA
SOURCE: Tetrahedron: Asymmetry (1997), 8(13), 2109-2114
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:190676
GI



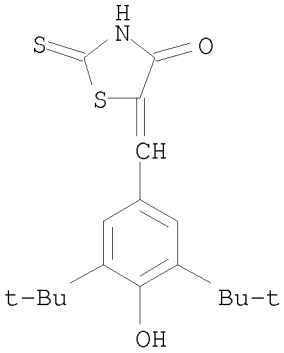
I

AB The kinetic resolution of tazofelone (I) has been reported. The resolution of this sulfide was accomplished via enantioselective sulfoxide formation with tert-Bu hydroperoxide in the presence of a chiral tartrate/titanium complex. The resolution was performed on analogs of compound I in order to explore the substrate specificity of the kinetic resolution These expts. have shown that the success of the enantioselective oxidation of this sulfide by tert-Bu hydroperoxide is greatly influenced by the nature of the neighboring amide functionality.

IT 67739-23-5 107902-67-0, Tazofelone
RL: RCT (Reactant); RACT (Reactant or reagent)
(kinetic resolution of tazofelone analogs via enantioselective oxidation)

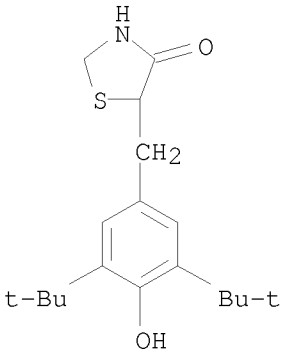
RN 67739-23-5 CAPLUS

CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]-2-thioxo- (CA INDEX NAME)



RN 107902-67-0 CAPLUS

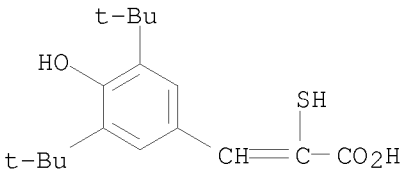
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]- (CA INDEX NAME)



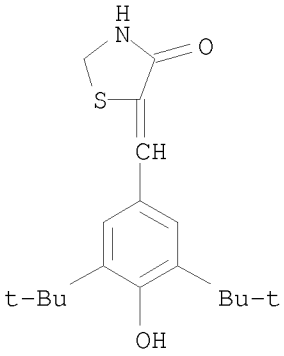
IT 107889-30-5P 107889-32-7P 107889-35-0P
132392-33-7P 192440-87-2P 194224-56-1P
194224-57-2P 194224-58-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(kinetic resolution of tazofelone analogs via enantioselective oxidation)

RN 107889-30-5 CAPLUS

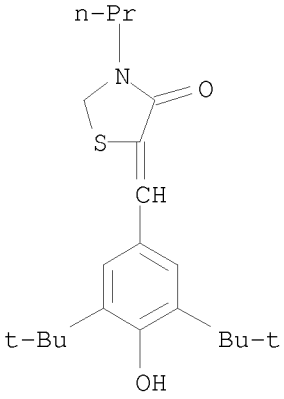
CN 2-Propenoic acid, 3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-mercapto- (CA INDEX NAME)



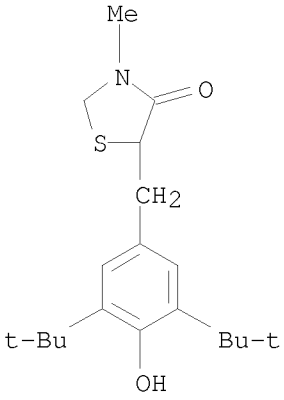
RN 107889-32-7 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]- (CA INDEX NAME)



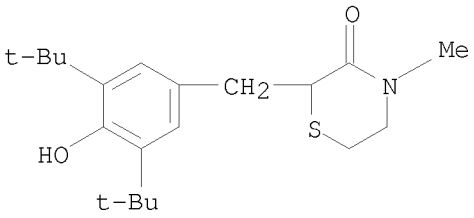
RN 107889-35-0 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]-3-propyl- (CA INDEX NAME)



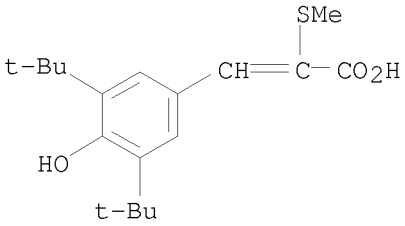
RN 132392-33-7 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-3-methyl- (CA INDEX NAME)



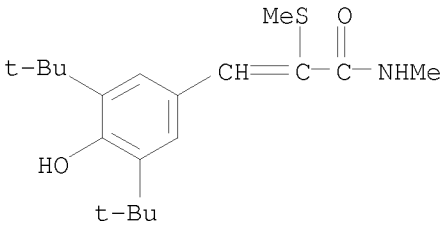
RN 192440-87-2 CAPLUS
CN 3-Thiomorpholinone, 2-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-4-methyl- (CA INDEX NAME)



RN 194224-56-1 CAPLUS
CN 2-Propenoic acid, 3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-(methylthio)- (CA INDEX NAME)

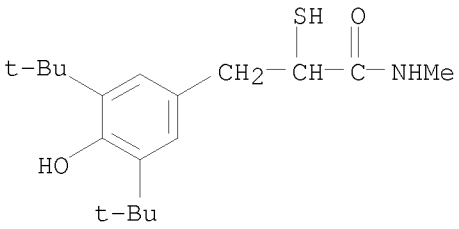


RN 194224-57-2 CAPLUS
CN 2-Propenamide, 3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-N-methyl-2-(methylthio)- (CA INDEX NAME)



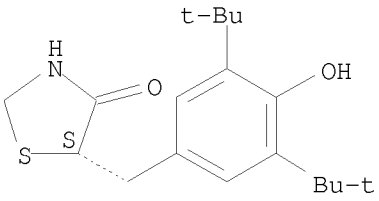
RN 194224-58-3 CAPLUS
CN Benzenepropanamide, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-mercapto-

N-methyl- (CA INDEX NAME)



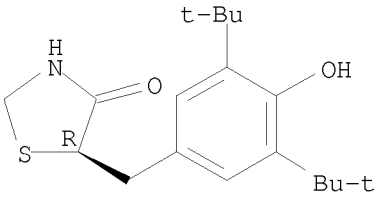
IT 136433-32-4P 136433-33-5P 136433-35-7P
    192440-88-3P 194224-55-0P 194224-59-4P
    RL: SPN (Synthetic preparation); PREP (Preparation)
       (kinetic resolution of tazofelone analogs via enantioselective oxidation)
RN 136433-32-4 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-,
    (5S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



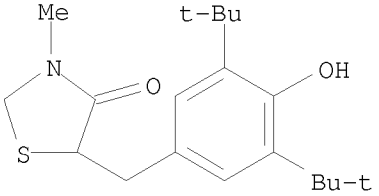
RN 136433-33-5 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-,
    (5R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 136433-35-7 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-3-
    methyl-, (-)- (CA INDEX NAME)

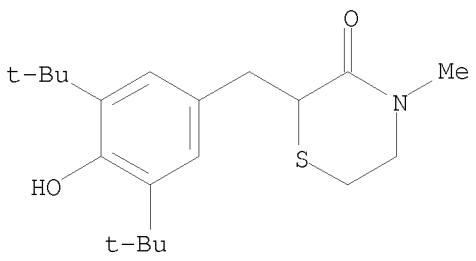
Rotation (-).



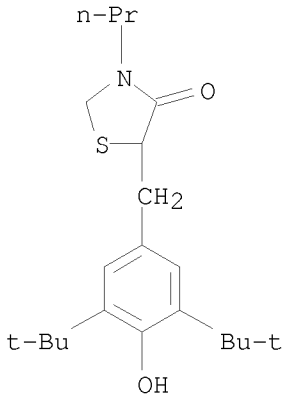
RN 192440-88-3 CAPLUS

CN 3-Thiomorpholinone, 2-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-4-methyl-, (-)- (CA INDEX NAME)

Rotation (-).

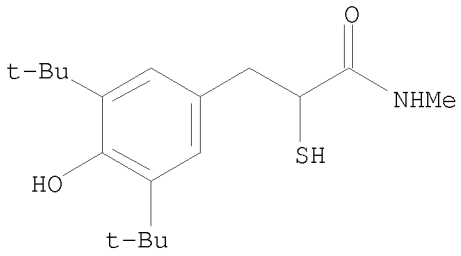


RN 194224-55-0 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-3-propyl- (CA INDEX NAME)



RN 194224-59-4 CAPLUS
CN Benzenepropanamide, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-mercapto-N-methyl-, (-)- (CA INDEX NAME)

Rotation (-).

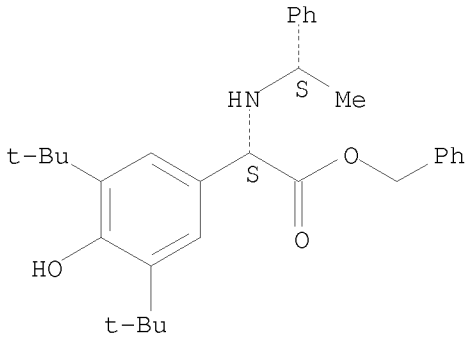


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 22 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:307083 CAPLUS
DOCUMENT NUMBER: 127:5324
ORIGINAL REFERENCE NO.: 127:1209a,1212a
TITLE: Chiral recognition by EPR and ENDOR spectroscopy via diastereomers

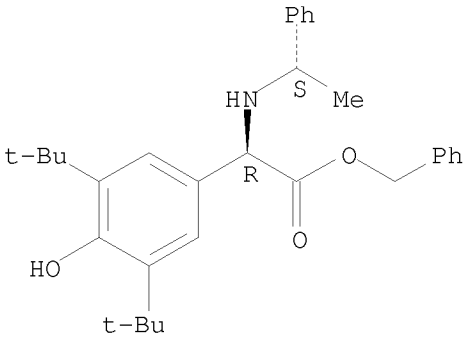
AUTHOR(S): Joerss, Elke; Schuler, Paul; Maichle-Moessmer, Caecilia; Abram, Sonja; Stegmann, Hartmut B.
CORPORATE SOURCE: University of Tubingen, Tubingen, D-72076, Germany
SOURCE: Enantiomer (1997), 2(1), 5-16
CODEN: EANTE2; ISSN: 1024-2430
PUBLISHER: Gordon & Breach
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Diastereomeric phenylglycine and phenylalanine derivs. 4,3,5-HO(Me3C)2C6H2CR(CO2R1)NHCHMePh [R = H, R1 = PhCH2, Me (2), Bu (3), R = Me, R1 = PhCH2 (4), Me (5)] were synthesized. The isomers were separated and then investigated by NMR and EPR/ENDOR spectroscopy. The absolute configurations of the two diastereomeric mols. 5, labeled A and B, were assigned by X-ray structure anal. Generally the diastereomers prepared show different NMR and EPR spectra. In the 1H-NMR spectra of compds. 2, 4, and 5 most signals of the A diastereomers are located at higher field than those of the corresponding B diastereomers. The EPR spectra of the A and B diastereomers of 2 and 3 differ in the β-H and nitrogen coupling consts., the A diastereomers show a smaller β-proton coupling constant Compds. 4 and 5 differ in the γ-H and nitrogen coupling consts. These results can be interpreted in terms of different low energy conformations of the diastereomers. The A diastereomers show stronger interactions between the phenol moiety and the rest of the mol.
IT 190271-94-4P 190271-98-8P 190272-01-6P
190272-06-1P 190272-09-4P 190272-12-9P
190272-16-3P 190272-21-0P 190272-25-4P
190272-29-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(chiral recognition by EPR and ENDOR spectroscopy via diastereomers)
RN 190271-94-4 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-[[(1S)-1-phenylethyl]amino]-, phenylmethyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



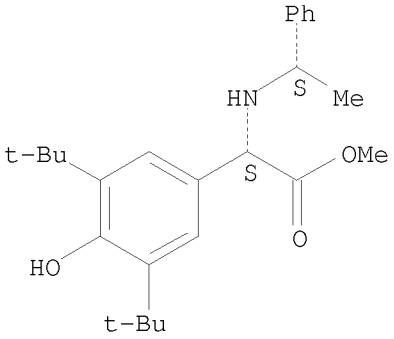
RN 190271-98-8 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-[[(1S)-1-phenylethyl]amino]-, phenylmethyl ester, (αR)- (CA INDEX NAME)

Absolute stereochemistry.



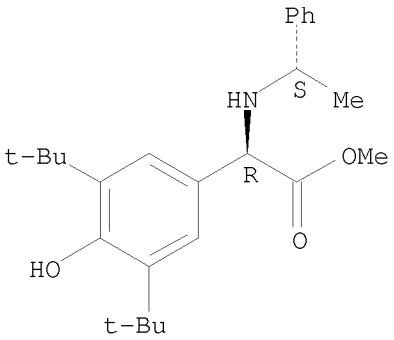
RN 190272-01-6 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-[[(1S)-1-phenylethyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



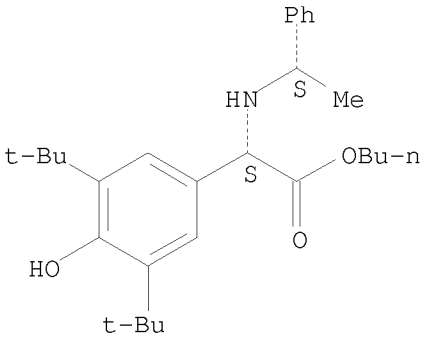
RN 190272-06-1 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-[[(1S)-1-phenylethyl]amino]-, methyl ester, (αR)- (CA INDEX NAME)

Absolute stereochemistry.



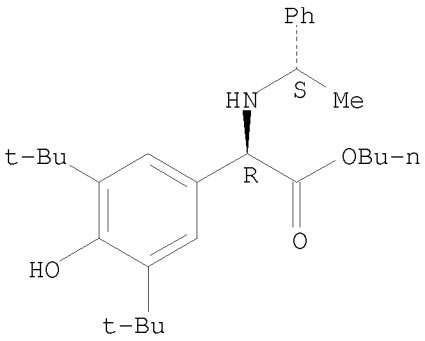
RN 190272-09-4 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-[[(1S)-1-phenylethyl]amino]-, butyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



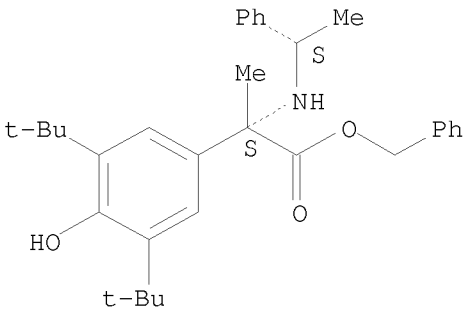
RN 190272-12-9 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-[[(1S)-1-phenylethyl]amino]-, butyl ester, (αR)- (CA INDEX NAME)

Absolute stereochemistry.



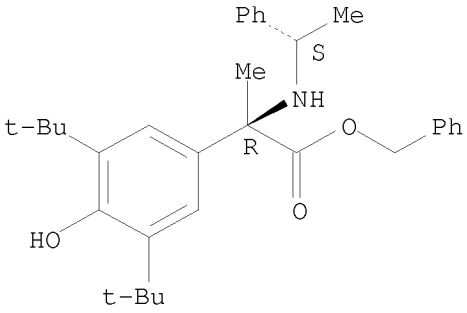
RN 190272-16-3 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl-α-[[(1S)-1-phenylethyl]amino]-, phenylmethyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



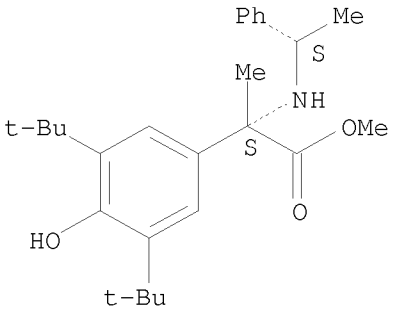
RN 190272-21-0 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl-α-[[(1S)-1-phenylethyl]amino]-, phenylmethyl ester, (αR)- (CA INDEX NAME)

Absolute stereochemistry.



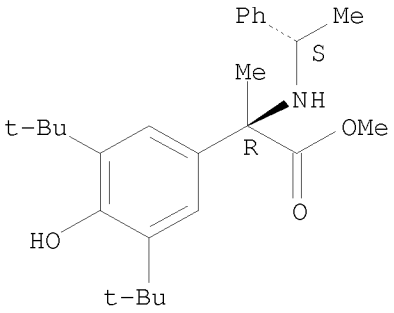
RN 190272-25-4 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl-α-[[(1S)-1-phenylethyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



RN 190272-29-8 CAPLUS
CN Benzeneacetic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl-α-[[(1S)-1-phenylethyl]amino]-, methyl ester, (αR)- (CA INDEX NAME)

Absolute stereochemistry.



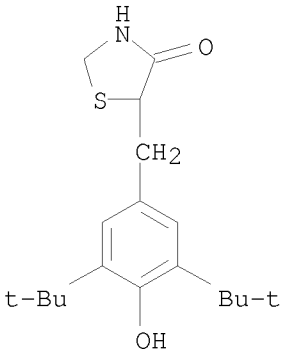
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 23 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:211885 CAPLUS
DOCUMENT NUMBER: 126:271730
ORIGINAL REFERENCE NO.: 126:52477a,52480a
TITLE: Chiral separation of neutral species by capillary electrophoresis. Evaluation of a theoretical model

AUTHOR(S): Surapaneni, S.; Ruterbories, K.; Lindstrom, T.
CORPORATE SOURCE: Drug Metabolism Disposition, Eli Lilly and Company, Indianapolis, IN, 46285, USA
SOURCE: Journal of Chromatography, A (1997), 761(1 + 2), 249-257
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A theor. model has been developed for the separation of enantiomers of neutral species by employing a combination of charged and neutral cyclodextrins. A neutral compound (LY213829), an ionizable cyclodextrin (sulfobutylether-cyclodextrin), and three neutral cyclodextrins (β-cyclodextrin, trimethyl-β-cyclodextrin, hydroxypropyl-β-cyclodextrin) were chosen to test the model. The model parameters were obtained by performing two specific sets of expts. Resolution and selectivity can be readily obtained from these model parameters. The validity of the model has been demonstrated by resolving enantiomers of LY213829 and its four isomeric sulfoxide metabolites, and the model was very successful in predicting the migration times and resolution of the LY213829 enantiomers. Baseline separation was achieved for all the analytes.

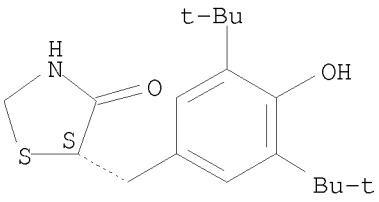
IT 107902-67-0, LY213829 136433-32-4 136433-33-5
189036-36-0, (S)-LY 262066 189036-40-6, (R)-LY 262066
189036-44-0, (S)-LY 262067 189036-48-4, (R)-LY 262067
RL: ANT (Analyte); ANST (Analytical study)
(chiral separation of neutral species (drugs and their metabolites) by capillary electrophoresis using cyclodextrins and evaluation of a theor. model)

RN 107902-67-0 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]- (CA INDEX NAME)



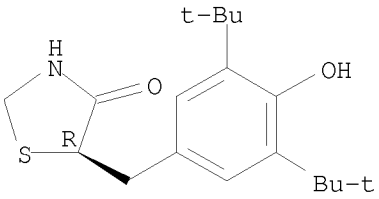
RN 136433-32-4 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, (5S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



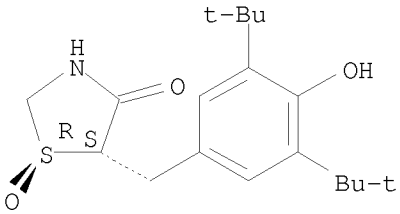
RN 136433-33-5 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, (5R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



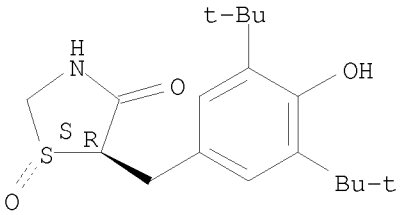
RN 189036-36-0 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, 1-oxide, (1R,5S)- (CA INDEX NAME)

Absolute stereochemistry.



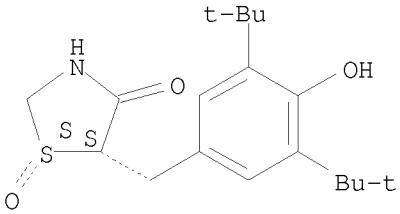
RN 189036-40-6 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, 1-oxide, (1S,5R)- (CA INDEX NAME)

Absolute stereochemistry.



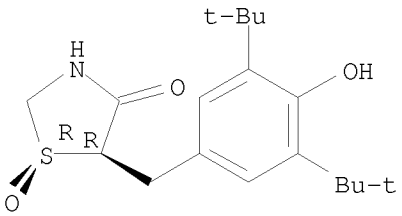
RN 189036-44-0 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, 1-oxide, (1S,5S)- (CA INDEX NAME)

Absolute stereochemistry.



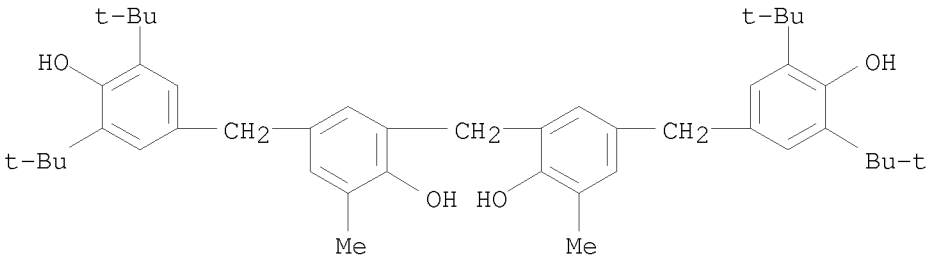
RN 189036-48-4 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, 1-oxide, (1R,5R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

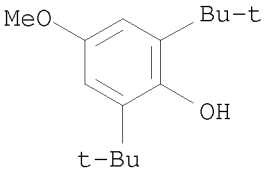
L5 ANSWER 24 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:25388 CAPLUS
DOCUMENT NUMBER: 124:175574
ORIGINAL REFERENCE NO.: 124:32551a,32554a
TITLE: Annelated Calixarenes Composed of Calix[4]arenes with Hydroxy Groups in the Endo and Exo Position
AUTHOR(S): Boehmer, Volker; Doerrenbaecher, Ralph; Frings, Michael; Heydenreich, Mathias; de Paoli, Diana; Vogt, Walter; Ferguson, George; Thondorf, Iris
CORPORATE SOURCE: Institut fuer Organische Chemie, Johannes Gutenberg Universitaet, Mainz, D-55099, Germany
SOURCE: Journal of Organic Chemistry (1996), 61(2), 549-59
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:175574
AB Various phenol-derived calix[4]arenes bearing four hydroxy groups in the exo position were prepared by uncatalyzed condensation of suitable dimers or tetramers with formaldehyde in xylene in yields up to 44%. A tetra-tert-Bu compound was shown by X-ray anal. to adopt a regular cone conformation (nearly identical in shape with the endo isomer) with two intramol. O-H···O hydrogen bonds, while the corresponding dimer (6c) prefers a conformation (not possible in the calixarene) with two intramol. O-H···π(arene) interactions. Condensation of exo-calix[4]arenes with free ortho positions (easily available by debutylation) with bisbromomethylated dimers gave annelated double and triple calixarenes consisting of endo- and exo-calix[4]arene structures. Mol. dynamics calcns. suggest that one exo-calixarene part in an annelated hydroxycalixarene is less mobile than an entirely flexible part in a corresponding monomeric hydroxycalixarene. A complete interconversion cone → cone is impossible, however, which enables the construction of inherently chiral mols.
IT 173974-50-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and conformation of annelated hydroxycalixarenes)
RN 173974-50-0 CAPLUS
CN Phenol, 2,2'-methylenebis[4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-6-methyl- (9CI) (CA INDEX NAME)



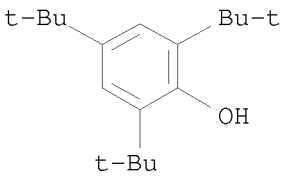
L5 ANSWER 25 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:57048 CAPLUS
DOCUMENT NUMBER: 122:10154
ORIGINAL REFERENCE NO.: 122:2257a,2260a
TITLE: The preparation of chiral titanium reagents: a comparison of new and known ligands
AUTHOR(S): Duthaler, Rudolf O.; Hafner, Andreas; Alsters, Paul L.; Bold, Guido; Rihs, Grety; Rothe-Streit, Petra; Wyss, Bernhard
CORPORATE SOURCE: Central Research Laboratories, CIBA, Postfach, Basle, CH-4002, Switz.
SOURCE: Inorganica Chimica Acta (1994), 222(1-2), 95-113
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Allyltitanium compds. and Ti enolates derived from monocyclopentadienylchlorotitanium complexes with two chiral alkoxy ligands add with high enantioface discrimination to aldehydes. While two diacetone-D-glucose ligands are perfectly suited for aldol reactions, tartrate derived 1,4-diol ligands, available in both enantiomeric forms, give high induction for the allyltitanation only. The chelating 1,4-diol ligands with a fixed C(2)-C(3) bond are rather insensitive to structural changes, as opposed to diacetone glucose, where only minor structural modifications at the acetal carbons are tolerated. Crucial for high enantioselectivity is apparently an interligand interaction, which can either be effected by a small Cp ligand and large Ph substituents or by a large pentamethyl Cp and small methyls. Expts. with new dibenzobicyclo[2.2.2]octane based 1,4-diol ligands show that the effect of intraligand strain on enantioselectivity is small in comparison with the impact of the interligand, Cp substituent, interaction. New x-ray evidence from the crystal structure anal. of a μ-oxo-bridged dimer shows that dioxolane-fixed seven-membered 1,3-dioxa-2-titanacycles are conformationally quite flexible. Explanations for the mechanism of asym. induction by these complexes, which are based on previous x-ray data, have therefore to be rated as less stringent than assumed before.

IT 489-01-0, 2,6-Di-tert-butyl-4-methoxyphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chiral titanium reagents and a comparison of new and known ligands)
RN 489-01-0 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-methoxy- (CA INDEX NAME)



L5 ANSWER 26 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:680575 CAPLUS
DOCUMENT NUMBER: 121:280575
ORIGINAL REFERENCE NO.: 121:51223a,51226a
TITLE: Stereoselective protonation of carbanions. 5. Effects of reaction conditions on the enantioselective protonation of lactone enolates
AUTHOR(S): Gerlach, Uwe; Haubenreich, Thomas; Huenig, Siegfried
CORPORATE SOURCE: Inst. Organische Chemie, Univ. Wuerzburg, Wuefrzburg, D-97074, Germany
SOURCE: Chemische Berichte (1994), 127(10), 1981-8
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Protonation of enolates derived from racemic 2,2-dimethyl-5-phenyl-1,3-dioxolan-4-one and 2,2-dimethyl-4-phenyl-1,3-oxathiolan-5-one by using standard conditions gave enantioselectivities up to 54 and 50% ee, resp., depending on the chiral proton source. The degrees of deuteration and enantioselectivity were not correlated. All results demonstrate the complexity of enantioselective protonation of enolatees which still need empirical optimization.
IT 732-26-3, 2,4,6-Tri-tert-butylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(reagent; stereoselective protonation of lactone enolates)
RN 732-26-3 CAPLUS
CN Phenol, 2,4,6-tris(1,1-dimethylethyl)- (CA INDEX NAME)



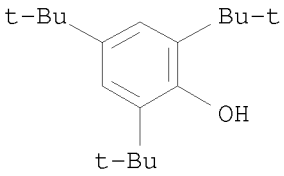
L5 ANSWER 27 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:408252 CAPLUS
DOCUMENT NUMBER: 121:8252
ORIGINAL REFERENCE NO.: 121:1776h,1777a
TITLE: Highly diastereoselective acetal cleavages using novel reagents prepared from organoaluminum and pentafluorophenol
AUTHOR(S): Ishihara, Kazuaki; Hanaki, Naoyuki; Yamamoto, Hisashi
CORPORATE SOURCE: Sch. Eng., Nagoya Univ., Nagoya, 464-01, Japan
SOURCE: Journal of the American Chemical Society (1993), 115(23), 10695-704
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:8252
AB Chiral acetals derived from aldehydes and (-)-(2R,4R)-2,4-pentanediol are cleaved selectively by organoaluminum reagents. The reaction proceeds via the retentive-alkylation process with >95% selectivities in most cases. Trialkylaluminum reagent is utilized for higher alkyl transfers, but for smaller alkyl transfers, a new reagent system, combining trialkylaluminum and halophenols such as pentafluorophenol or 2,4,6-trichlorophenol, is employed. Chiral acetals derived from aldehydes and 1,3-butanediol are cleaved selectively by trialkylaluminum, even for small alkyl transfers. Oxetane is also

exposed to these aluminum reagents, and the retentive-alkylation products are obtained stereoselectively. The reaction of acetals derived from (-)-(2R,4R)-2,4-pentanediol and ketones in the presence of a catalytic amount of aluminum pentafluorophenoxide produces reductively cleaved products with high diastereoselectivity. The reaction is a new means of diastereoselective cleavage of acetals: an intramol. Meerwein-Ponndorf-Verley reductive and Oppenauer oxidative reaction on an acetal template.

IT 732-26-3, 2,4,6-Tri-tert-butylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(reagent from alkylaluminums and, for diastereoselective cleavage of chiral acetals)

RN 732-26-3 CAPLUS

CN Phenol, 2,4,6-tris(1,1-dimethylethyl)- (CA INDEX NAME)



L5 ANSWER 28 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:313944 CAPLUS

DOCUMENT NUMBER: 120:313944

ORIGINAL REFERENCE NO.: 120:54941a,54944a

TITLE: Chiral recognition by proton-NMR, EPR, and ENDOR spectroscopy

AUTHOR(S): Stegmann, Hartmut B.; Maeurer, Manfred; Hoefler, Ulrike; Scheffler, Klaus; Hewgill, Frank

CORPORATE SOURCE: Inst. Org. Chem., Univ. Tuebingen, Tuebingen, 72076, Germany

SOURCE: Chirality (1993), 5(4), 282-7
CODEN: CHRLEP; ISSN: 0899-0042

DOCUMENT TYPE: Journal

LANGUAGE: English

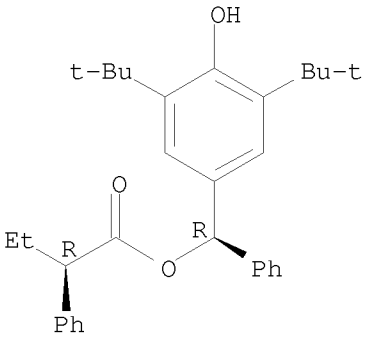
AB Chiral recognition with magnetic methods requires the formation of diastereomers. Due to the variety of appropriate reactions, hydrogen bond formation, esterification, and acetalization as well as host-guest interactions were chosen for basic investigations. The results obtained indicate that in the case of diamagnetic compds. the chemical shifts and for paramagnetic compds. the β-proton coupling consts. are the most useful parameters. By combination of both pieces of information, assignment of the absolute configuration was achieved.

IT 126504-48-1P 126504-49-2P 126504-50-5P
126504-51-6P 154974-51-3P 155074-27-4P
155074-28-5P 155074-29-6P 155074-30-9P
RL: PREP (Preparation)
(formation and chiral recognition of, by NMR EPR and ENDOR spectroscopy)

RN 126504-48-1 CAPLUS

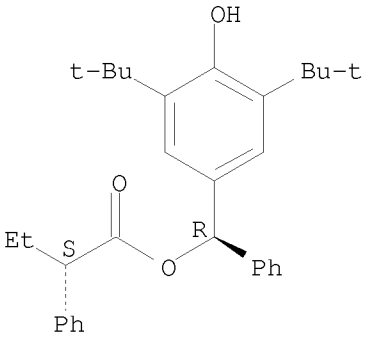
CN Benzeneacetic acid, α-ethyl-, (R)-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]phenylmethyl ester, (αR)-rel- (CA INDEX NAME)

Relative stereochemistry.



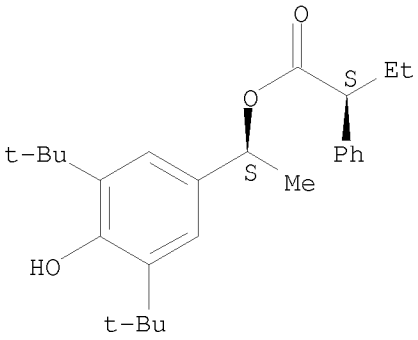
RN 126504-49-2 CAPLUS
CN Benzeneacetic acid, α-ethyl-,
(R)-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]phenylmethyl ester,
(αS)-rel- (CA INDEX NAME)

Relative stereochemistry.



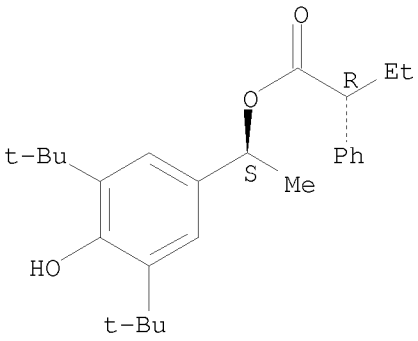
RN 126504-50-5 CAPLUS
CN Benzeneacetic acid, α-ethyl-,
(1R)-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]ethyl ester,
(αR)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 126504-51-6 CAPLUS
CN Benzeneacetic acid, α-ethyl-,
(1R)-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]ethyl ester,
(αS)-rel- (CA INDEX NAME)

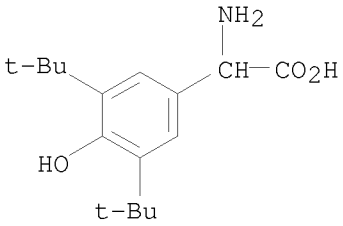
Relative stereochemistry.



RN 154974-51-3 CAPLUS
CN 1,4,7,10,13,16-Hexaoxacyclooctadecane-2,3,11,12-tetracarboxylic acid, (2R,3R,11R,12R)-, compd. with α-amino-3,5-bis(1,1-dimethylethyl)-4-hydroxybenzeneacetic acid (1:1) (CA INDEX NAME)

CM 1

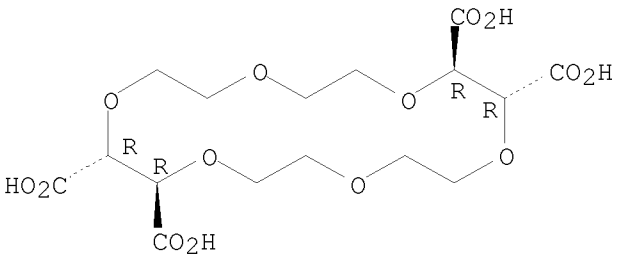
CRN 65559-23-1
CMF C16 H25 N O3



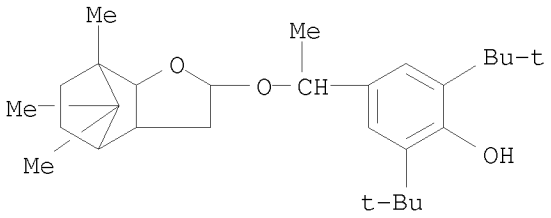
CM 2

CRN 61696-54-6
CMF C16 H24 O14

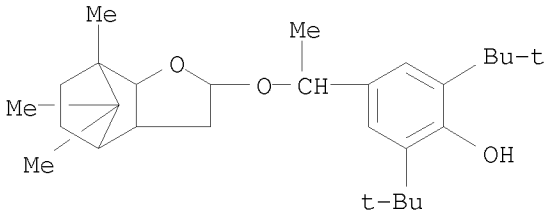
Absolute stereochemistry. Rotation (+).



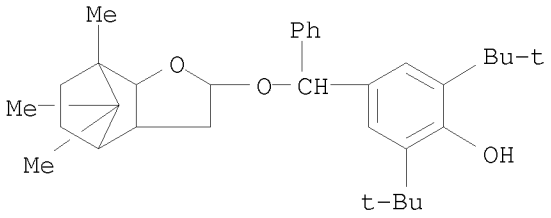
RN 155074-27-4 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[1-[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]ethyl]-, [2α(S*),3aβ,4β,7β,7aβ]- (9CI) (CA INDEX NAME)



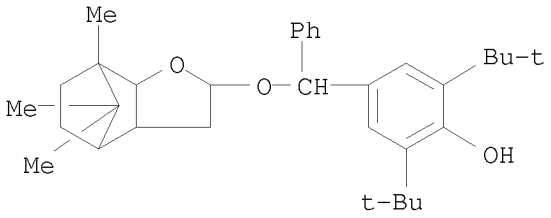
RN 155074-28-5 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[1-[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]ethyl]-, [2α(R*),3aβ,4β,7β,7aβ]- (9CI) (CA INDEX NAME)



RN 155074-29-6 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]phenylmethyl]-, [2α(S*),3aβ,4β,7β,7aβ]- (9CI) (CA INDEX NAME)

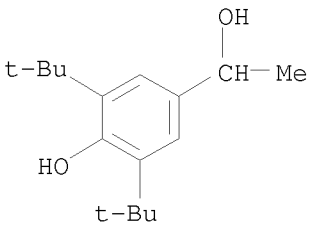


RN 155074-30-9 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]phenylmethyl]-, [2α(R*),3aβ,4β,7β,7aβ]- (9CI) (CA INDEX NAME)

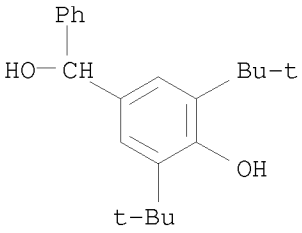


IT 14681-20-0 20017-39-4
RL: PRP (Properties)
(reaction with phenylbutyryl chloride and benzofuranol, chiral recognition of diastereomers formed from, by magnetic methods)
RN 14681-20-0 CAPLUS

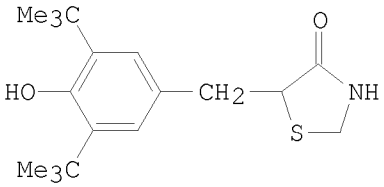
CN Benzenemethanol, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl- (CA INDEX NAME)



RN 20017-39-4 CAPLUS
CN Benzenemethanol, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-phenyl- (CA INDEX NAME)



L5 ANSWER 29 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:86234 CAPLUS
DOCUMENT NUMBER: 120:86234
ORIGINAL REFERENCE NO.: 120:15269a,15272a
TITLE: NMR studies of drugs. Applications of achiral and chiral lanthanide shift reagents to a 5-substituted-4-thiazolidinone
AUTHOR(S): Roberts, Katherine; Rothchild, Robert; Wyss, Helen
CORPORATE SOURCE: John Jay Coll. Crim. Justice, City Univ. New York, New York, NY, 10019-1199, USA
SOURCE: Spectroscopy Letters (1993), 26(10), 1901-21
CODEN: SPLEBX; ISSN: 0038-7010
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

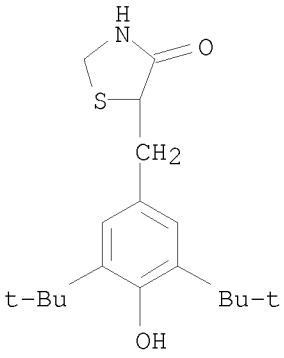
AB The 60 MHz 1H NMR spectra of racemic LY-213829 (I), have been studied in CDCl3 solution at 28° with the achiral lanthanide shift reagent (LSR), tris(6,6,7,7,8,8,8-heptafluoro-2,2-dimethyl-3,5-octanedionato)europium(III), and the chiral LSRs, tris[3-(heptafluoropropylhydroxymethylene)-(+)-camphorato]europium(III) (II) and tris[3-(trifluoromethylhydroxymethylene)-(+)-

camphorato]europium(III). Significant enantiomeric shift differences were observed in the presence of added II for the aryl protons of I that should permit direct determination of enantiomeric excess. Relative magnitudes of lanthanide-induced shift for the different nuclei of I with the three LSRs are compared and discussed in terms of preferred LSR binding sites. A favored conformation of I1 with respect to rotation about the C(5)-CH2 bond is suggested.

IT 107902-67-0, LY 213829
RL: PRP (Properties)
(NMR of, achiral and chiral lanthanide shift reagents in)

RN 107902-67-0 CAPLUS

CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]- (CA INDEX NAME)



L5 ANSWER 30 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN

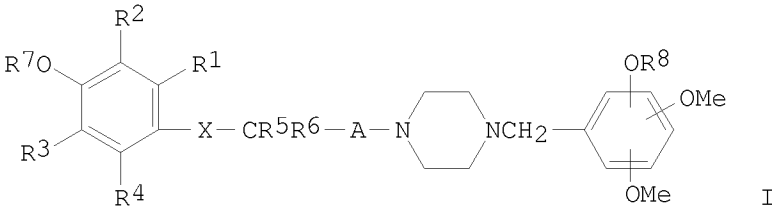
ACCESSION NUMBER: 1993:472628 CAPLUS
DOCUMENT NUMBER: 119:72628
ORIGINAL REFERENCE NO.: 119:13097a,13100a
TITLE: Preparation of trimetazidine derivatives and pharmaceutical compositions containing them, for treatment of ischemic myocardium and peripheral vascular pathologies
INVENTOR(S): Regnier, Gilbert; Vilaine, Jean Paul; Villeneuve, Nicole; Bidouard, Jean Pierre; Iliou, Jean Pierre; Lenaers, Albert
PATENT ASSIGNEE(S): ADIR et Cie., Fr.
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 533579	A1	19930324	EP 1992-402566	19920918
EP 533579	B1	19961204		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
FR 2681324	A1	19930319	FR 1991-11469	19910918
FR 2681324	B1	19931029		
CA 2078520	A1	19930319	CA 1992-2078520	19920917
CA 2078520	C	20010424		
AU 9224537	A	19930325	AU 1992-24537	19920917
AU 647964	B2	19940331		
US 5283246	A	19940201	US 1992-946933	19920917
ZA 9207165	A	19930324	ZA 1992-7165	19920918
JP 05194451	A	19930803	JP 1992-293636	19920918

JP 06076396	B	19940928			
AT 145899	T	19961215	AT 1992-402566		19920918
ES 2097299	T3	19970401	ES 1992-402566		19920918
PRIORITY APPLN. INFO.:			FR 1991-11469	A	19910918

OTHER SOURCE(S): MARPAT 119:72628

GI



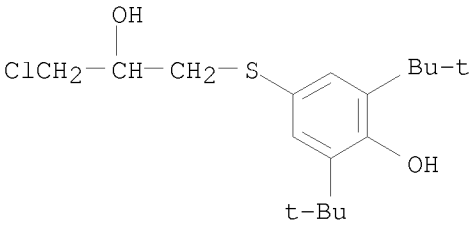
I

AB Title compds. I [R1, R4 (same or different) = H, Me, MeO; R2, R3 (same or different) = linear or branched C1-6 alkyl or alkoxy; R5, R6 (same or different) = H, Me; R7 = H, R7'CO (R7' = linear or branched C1-5 alkyl, Ph or PhCH2 (un)substituted at the Ph group by linear or branched C1-5 alkyl or alkoxy); R8 = H, linear or branched C1-5 alkyl; X = single bond, O, S; where X = O, S, then R1, R5 may be CH2; A = linear or branched C2-6 hydrocarbon chain (un)substituted by OH, where A may contain a chiral C] are prepared by condensation of an N-benzylpiperidine derivative with an appropriate tosyloxy derivative Compds. I, their salts, enantiomers, diastereoisomers, and pharmaceutical compns. containing them are also claimed. Biol. studies show that compds. I are useful for the treatment of ischemic myocardium and peripheral vascular pathologies.

IT 53690-11-2P 148089-88-7P 148089-89-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate to trimetazidine derivs.)

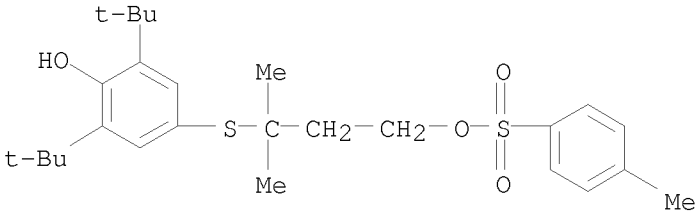
RN 53690-11-2 CAPLUS

CN Phenol, 4-[(3-chloro-2-hydroxypropyl)thio]-2,6-bis(1,1-dimethylethyl)- (CA INDEX NAME)

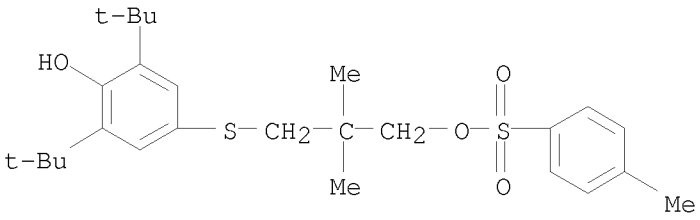


RN 148089-88-7 CAPLUS

CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[1,1-dimethyl-3-[[(4-methylphenyl)sulfonyl]oxy]propyl]thio]- (CA INDEX NAME)

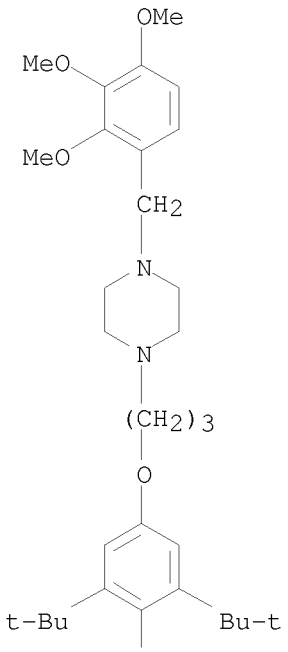


RN 148089-89-8 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[2,2-dimethyl-3-[[(4-methylphenyl)sulfonyl]oxy]propyl]thio]- (CA INDEX NAME)



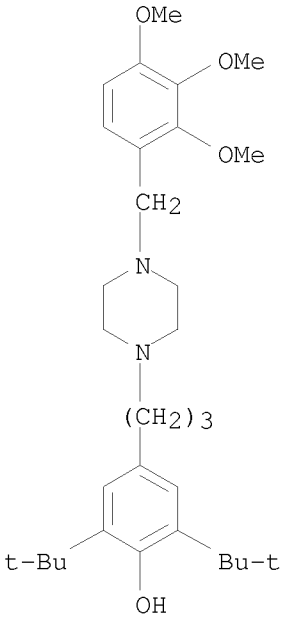
IT 148070-68-2P 148070-69-3P 148070-70-6P
148089-65-0P 148089-66-1P 148089-67-2P
148089-68-3P 148089-69-4P 148089-70-7P
148089-71-8P 148089-72-9P 148089-75-2P
148913-54-6P 148913-55-7P 148913-56-8P
148913-57-9P 148913-60-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for treatment of ischemic myocardium and peripheral vascular diseases)

RN 148070-68-2 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[3-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]propoxy]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

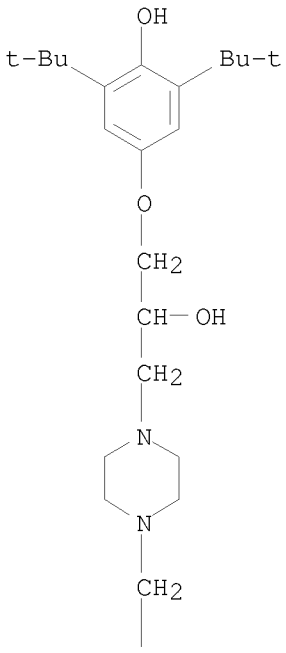
RN 148070-69-3 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[3-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]propyl]-, hydrochloride (1:2) (CA INDEX NAME)



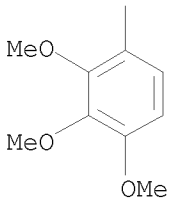
● 2 HCl

RN 148070-70-6 CAPLUS
CN 1-Piperazineethanol, α-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenoxy]methyl]-4-[(2,3,4-trimethoxyphenyl)methyl]-, hydrochloride (1:2) (CA INDEX NAME)

PAGE 1-A



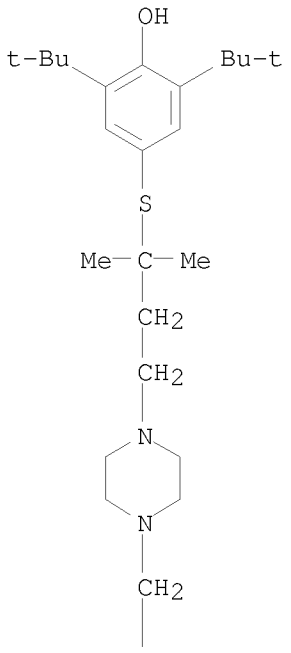
PAGE 2-A



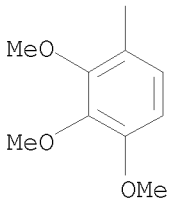
● 2 HCl

RN 148089-65-0 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[1,1-dimethyl-3-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]propyl]thio]- (CA INDEX NAME)

PAGE 1-A

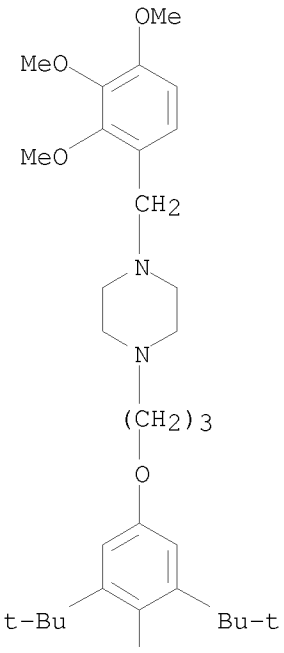


PAGE 2-A



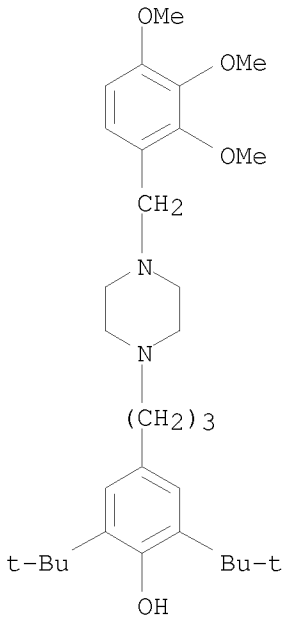
RN 148089-66-1 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[3-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]propoxy]- (CA INDEX NAME)

PAGE 1-A



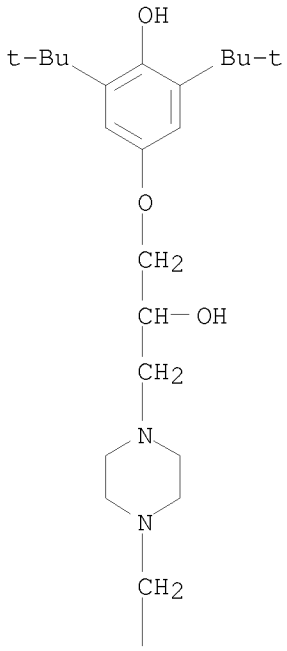
PAGE 2-A

RN 148089-67-2 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[3-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]propyl]- (CA INDEX NAME)

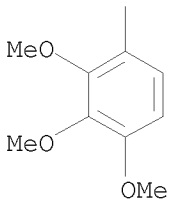


RN 148089-68-3 CAPLUS
CN 1-Piperazineethanol, α-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenoxy]methyl]-4-[(2,3,4-trimethoxyphenyl)methyl]- (CA INDEX NAME)

PAGE 1-A

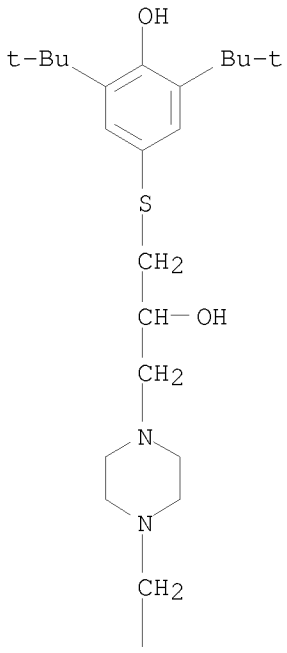


PAGE 2-A

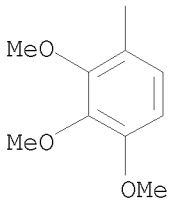


RN 148089-69-4 CAPLUS
CN 1-Piperazineethanol, α-[[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]methyl]-4-[(2,3,4-trimethoxyphenyl)methyl]- (CA INDEX NAME)

PAGE 1-A

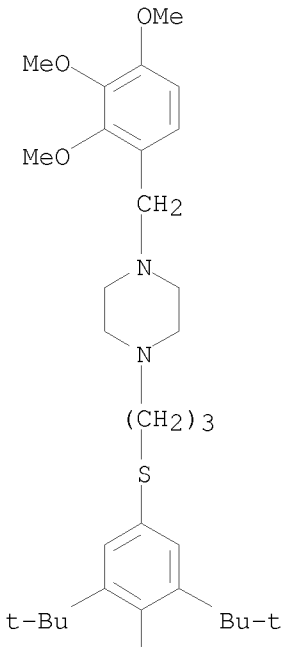


PAGE 2-A



RN 148089-70-7 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[3-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]propyl]thio]- (CA INDEX NAME)

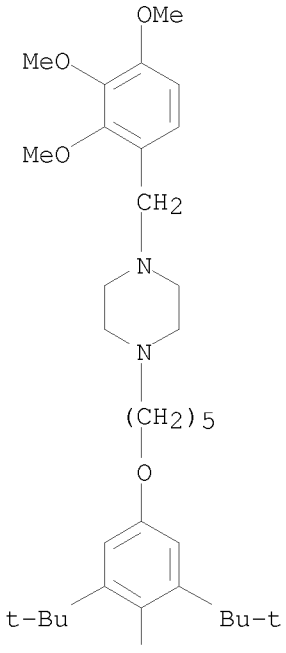
PAGE 1-A



PAGE 2-A

RN 148089-71-8 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[5-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]pentyl]oxy]- (CA INDEX NAME)

PAGE 1-A

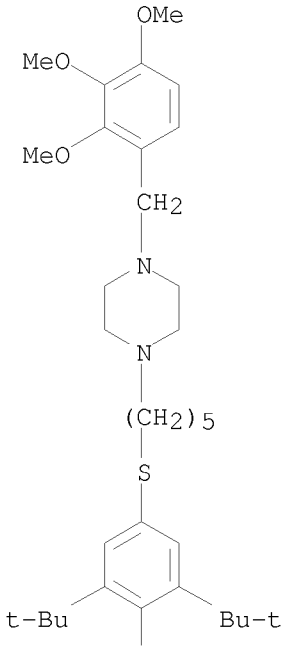


PAGE 2-A

OH

RN 148089-72-9 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[5-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]pentyl]thio]- (CA INDEX NAME)

PAGE 1-A

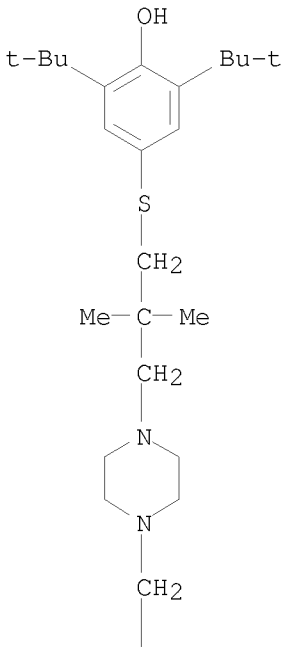


PAGE 2-A

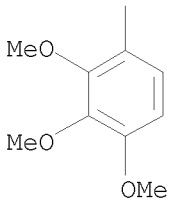
OH

RN 148089-75-2 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[2,2-dimethyl-3-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]propyl]thio]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

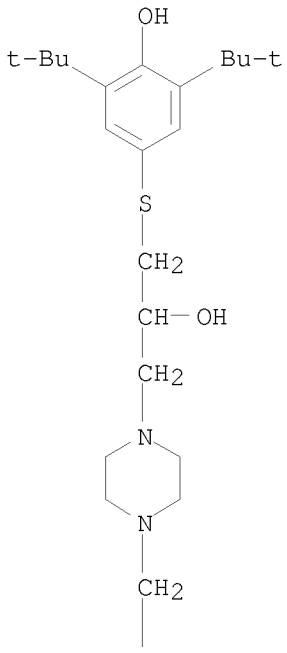


RN 148913-54-6 CAPLUS
CN 1-Piperazineethanol, α-[[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]methyl]-4-[(2,3,4-trimethoxyphenyl)methyl]-, (2E)-2-butenedioate (1:2) (salt) (9CI) (CA INDEX NAME)

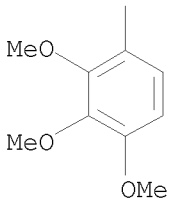
CM 1

CRN 148089-69-4
CMF C31 H48 N2 O5 S

PAGE 1-A



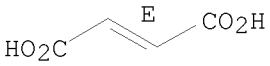
PAGE 2-A



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

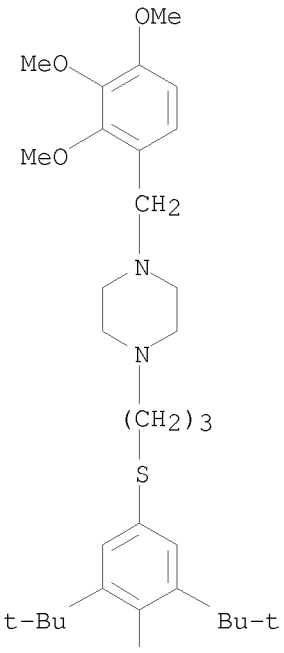


RN 148913-55-7 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[3-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]propyl]thio]-, (2E)-2-butenedioate (1:2) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 148089-70-7
CMF C31 H48 N2 O4 S

PAGE 1-A

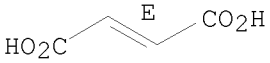


PAGE 2-A

CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

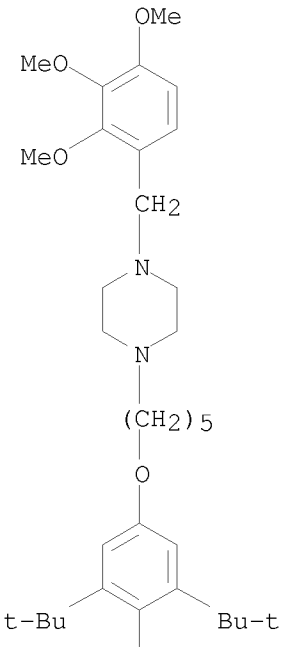


RN 148913-56-8 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[5-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]pentyl]oxy]-, (2E)-2-butenedioate (1:2) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 148089-71-8
CMF C33 H52 N2 O5

PAGE 1-A

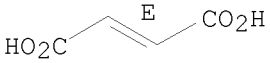


PAGE 2-A

CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

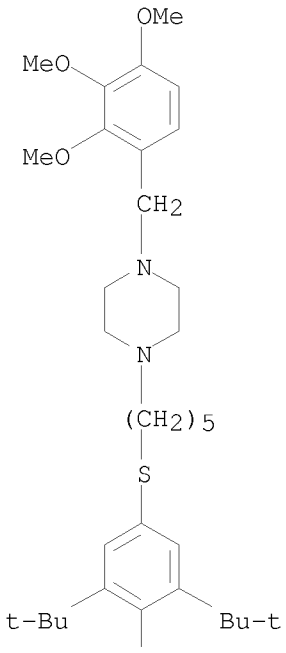


RN 148913-57-9 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[5-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]pentyl]thio]-, (2E)-2-butenedioate (1:2) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 148089-72-9
CMF C33 H52 N2 O4 S

PAGE 1-A

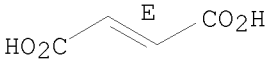


PAGE 2-A

CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

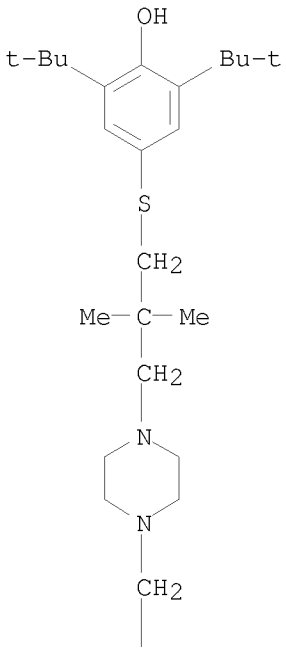


RN 148913-60-4 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[2,2-dimethyl-3-[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]propyl]thio]-, (2E)-2-butenedioate (1:2) (salt) (9CI) (CA INDEX NAME)

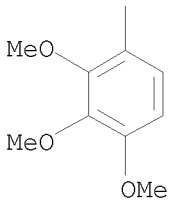
CM 1

CRN 148089-75-2
CMF C33 H52 N2 O4 S

PAGE 1-A



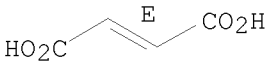
PAGE 2-A



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



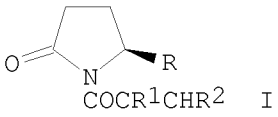
L5 ANSWER 31 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:592341 CAPLUS
DOCUMENT NUMBER: 117:192341
ORIGINAL REFERENCE NO.: 117:33251a,33254a
TITLE: Process for the production of (S)-vinyl and (S)-allenyl GABA
INVENTOR(S): Evans, Jonathan C.
PATENT ASSIGNEE(S): Merrell Dow Pharmaceuticals, Inc., USA
SOURCE: Eur. Pat. Appl., 50 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 492350	A1	19920701	EP 1991-121554	19911216
EP 492350	B1	19971015		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AU 9189635	A	19920618	AU 1991-89635	19911212
AU 644919	B2	19931223		
IL 100360	A	19980816	IL 1991-100360	19911212
CA 2057699	A1	19920618	CA 1991-2057699	19911216
CA 2057699	C	20021029		
HU 63829	A2	19931028	HU 1991-3969	19911216
HU 218793	B	20001228		
AT 159246	T	19971115	AT 1991-121554	19911216
ES 2110974	T3	19980301	ES 1991-121554	19911216
JP 04334364	A	19921120	JP 1991-352847	19911217
JP 3143877	B2	20010307		
US 5208345	A	19930504	US 1992-938661	19920831
AU 9453900	A	19940317	AU 1994-53900	19940121
AU 658538	B2	19950413		

PRIORITY APPLN. INFO.: US 1990-628738 A 19901217
US 1991-782941 B1 19911025

OTHER SOURCE(S): MARPAT 117:192341
GI



I

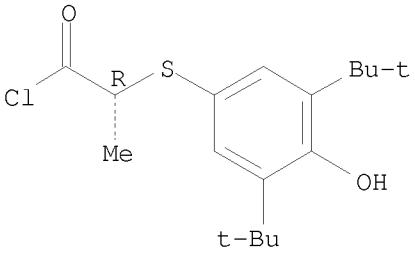
AB Title compds. were prepared from vinyl- or allenylpyrrolidone via acyl derivs. (2'S)-I (R = vinyl, allenyl; R1 = OSiMe2CMe3, R2 = H, Ph; R1 = OCH2Ph, 2-naphthylmethoxy, R2 = H) and (2'R)-I [R = vinyl, allenyl; R1 = 3,5-(Me3C)2C6H3O, 2,4-(Me3C)2C6H3O, 4,3,5-HO(Me3C)2C6H2S, R2 = H]. Thus, (2S)-lactic acid was silylated, converted to the acid chloride and used to acylate 5-vinylpyrrolidone. The resulting (2'S)-I (R = vinyl, R1 = Me3CSiMe2O, R2 = H) was hydrolyzed to give (4S)-CH2:CHCH(NH2)CH2CH2CO2H.

IT 143418-06-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation by, of vinylpyrrolidone)

RN 143418-06-8 CAPLUS

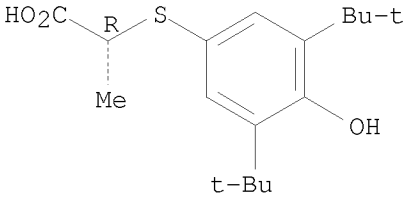
CN Propanoyl chloride, 2-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



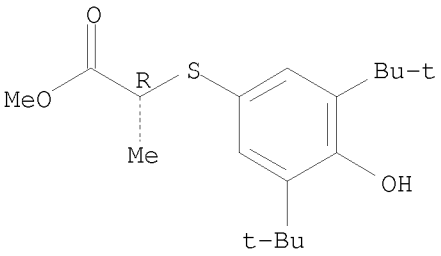
IT 143418-05-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)
RN 143418-05-7 CAPLUS
CN Propanoic acid, 2-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



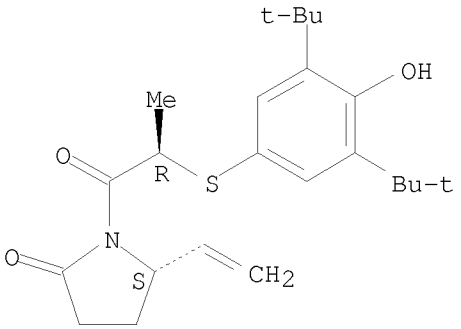
IT 143418-04-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ester hydrolysis of)
RN 143418-04-6 CAPLUS
CN Propanoic acid, 2-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

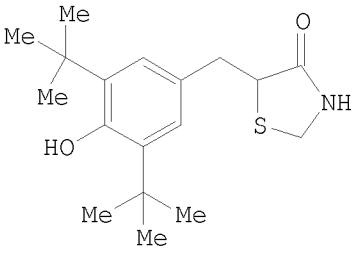


IT 143418-07-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 143418-07-9 CAPLUS
CN 2-Pyrrolidinone, 1-[2-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-oxopropyl]-5-ethenyl-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



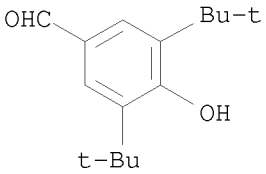
L5 ANSWER 32 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:448390 CAPLUS
DOCUMENT NUMBER: 117:48390
ORIGINAL REFERENCE NO.: 117:8630h,8631a
TITLE: Kinetic resolution of a racemic sulfide by enantioselective sulfoxide formation
AUTHOR(S): Phillips, Michael L.; Berry, Donnis M.; Panetta, Jill A.
CORPORATE SOURCE: Lilly Corp. Cent., Eli Lilly and Co., Indianapolis, IN, 46285, USA
SOURCE: Journal of Organic Chemistry (1992), 57(14), 4047-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

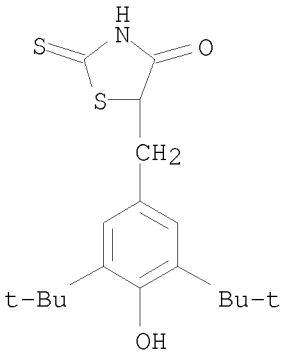
AB (±) 5-[[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-4-thiazolidinone (I) is a member of a series of compds. which has demonstrated efficacy in animal models of inflammatory bowel disease. A method of producing the individual enantiomers of this compound was required to allow comparative efficacy, pharmacokinetic and toxicol. studies to be undertaken. Kinetic resolution of this racemic sulfide I was achieved by incomplete oxidation to the sulfoxide with tert-Bu hydroperoxide in the presence of a chiral catalyst prepared from diisopropyl tartrate, titanium tetraisopropoxide and water. The reaction conditions were varied in an attempt to improve the enantiomeric excess (ee) of the unreacted sulfide. The recovered sulfide had an ee of 94% when the reaction was allowed to go to 79% completion.

IT 1620-98-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with rhodanine)
RN 1620-98-0 CAPLUS
CN Benzaldehyde, 3,5-bis(1,1-dimethylethyl)-4-hydroxy- (CA INDEX NAME)

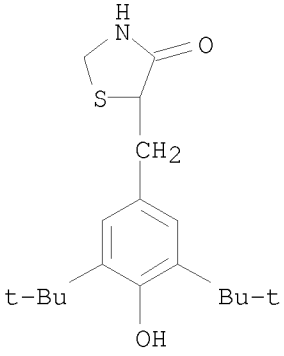


IT 107902-68-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desulfurization of)
RN 107902-68-1 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-2-

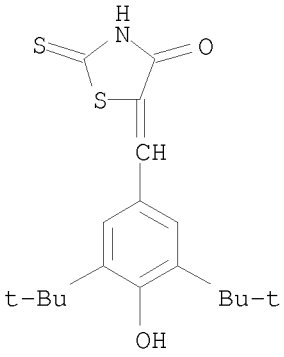
thioxo- (CA INDEX NAME)



IT 107902-67-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetic resolution of, by enantioselective oxidation of sulfide)
RN 107902-67-0 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]- (CA INDEX NAME)

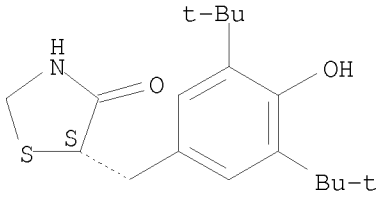


IT 67739-23-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 67739-23-5 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]-2-thioxo- (CA INDEX NAME)



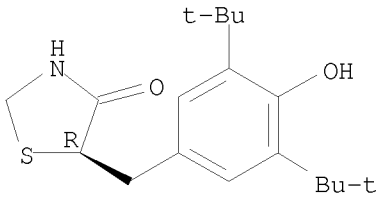
IT 136433-32-4 136433-33-5
RL: PROC (Process)
(separation of, from enantiomer)
RN 136433-32-4 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, (5S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

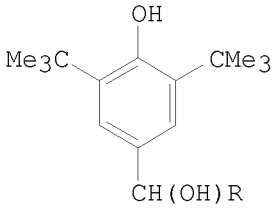


RN 136433-33-5 CAPLUS
CN 4-Thiazolidinone, 5-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-, (5R)- (CA INDEX NAME)

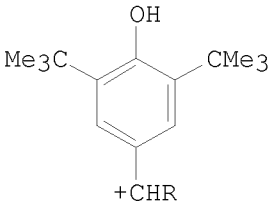
Absolute stereochemistry. Rotation (+).



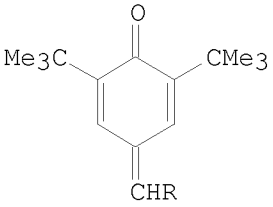
L5 ANSWER 33 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:213898 CAPLUS
DOCUMENT NUMBER: 116:213898
ORIGINAL REFERENCE NO.: 116:36229a,36232a
TITLE: Stereoelectronic and steric effects in the synthesis and recognition of diastereomeric ethers by NMR and EPR spectroscopy
AUTHOR(S): Maeurer, Manfred; Hiller, Wolfgang; Mueller, Bernd; Stegmann, Hartmut B.
CORPORATE SOURCE: Inst. Org. Chem., Univ. Tuebingen, Tuebingen, W-7400, Germany
SOURCE: Chemische Berichte (1992), 125(4), 857-65
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:213898
GI



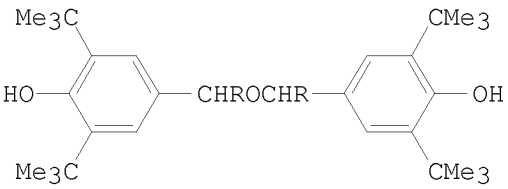
I



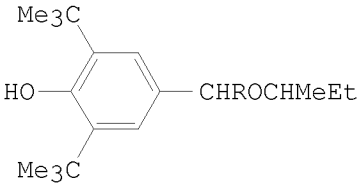
II



III



IV



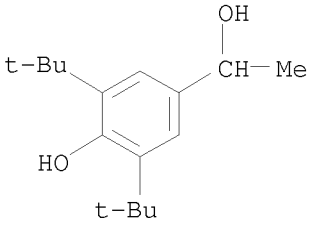
V

AB Carbinols I (R = Me, Et, CMe3) are easily dehydrated in the presence of catalytic amts. of a mineral acid to form carbocations (II), which can be reversibly deprotonated to the quinone methides (III). Therefore, an equilibrium between I and III is assumed. In the absence of nucleophiles, a reaction of II with I leads to sym. ethers (IV). In alc. solution, the solvent acts as a nucleophilic compound and the formation of an unsym. ether (V) is observed predominantly. If the nucleophile contains a chiral carbon atom, diastereomers are formed in this reaction and are observed in variable concns., depending on the reaction time. The assignment of these isomers to the meso and racemic compound has been achieved by NMR investigations in solution along with x-ray crystallog. The results indicate a remarkable thermodn. stabilization of the sym. ethers in the racemic form whereas the meso compds. are favored if the products are formed under kinetic control. In both cases the diastereomer ratio is determined by steric repulsion and the generalized anomeric effect. A bonding interaction of lone pairs of the ether oxygen with the π system of the corresponding phenoxyl ring was also observed by ESR. This electron delocalization contributes remarkably to the mechanism responsible for the distinction of the diastereomeric radicals by different β-proton coupling consts.

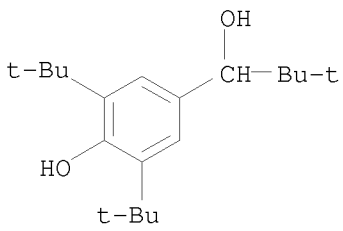
IT 14681-20-0 15018-01-6 20017-35-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydration of, equilibrium of)

RN 14681-20-0 CAPLUS

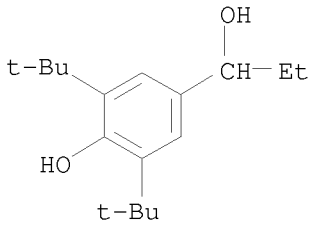
CN Benzenemethanol, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl- (CA INDEX NAME)



RN 15018-01-6 CAPLUS
CN Benzenemethanol, α,3,5-tris(1,1-dimethylethyl)-4-hydroxy- (CA INDEX NAME)

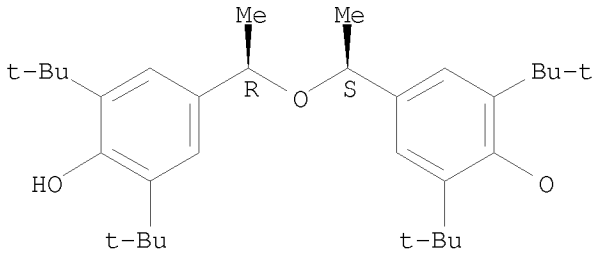


RN 20017-35-0 CAPLUS
CN Benzenemethanol, 3,5-bis(1,1-dimethylethyl)-α-ethyl-4-hydroxy- (CA INDEX NAME)



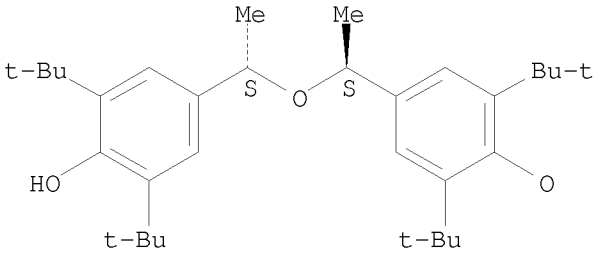
IT 138694-88-9P 138694-89-0P 138694-98-1P
138694-99-2P 138695-02-0P 138695-03-1P
RL: PRP (Properties); FORM (Formation, nonpreparative); PREP (Preparation)
(formation and ESR of)
RN 138694-88-9 CAPLUS
CN Phenoxy, 4-[1-[1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]ethoxy]ethyl]-2,6-bis(1,1-dimethylethyl)-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



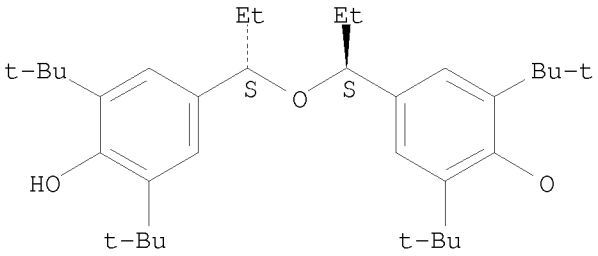
RN 138694-89-0 CAPLUS
CN Phenoxy, 4-[1-[1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]ethoxy]ethyl]-2,6-bis(1,1-dimethylethyl)-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



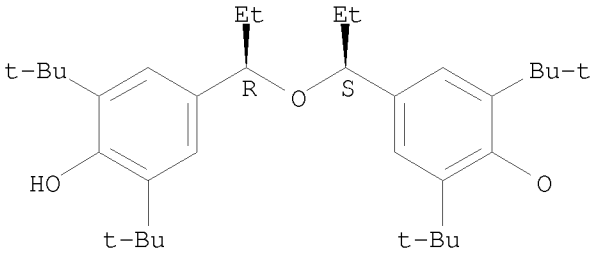
RN 138694-98-1 CAPLUS
CN Phenoxy, 4-[1-[1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]propoxy]propyl]-2,6-bis(1,1-dimethylethyl)-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



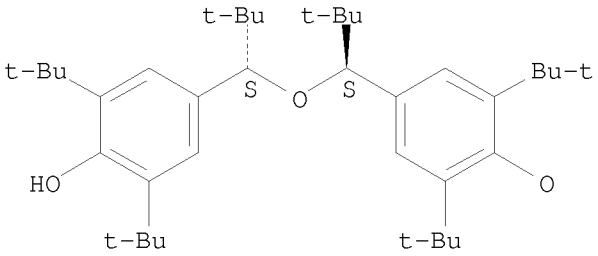
RN 138694-99-2 CAPLUS
CN Phenoxy, 4-[1-[1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]propoxy]propyl]-2,6-bis(1,1-dimethylethyl)-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



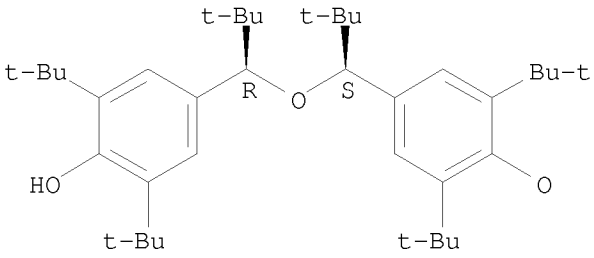
RN 138695-02-0 CAPLUS
CN Phenoxy, 4-[1-[1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2,2-dimethylpropoxy]-2,2-dimethylpropyl]-2,6-bis(1,1-dimethylethyl)-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

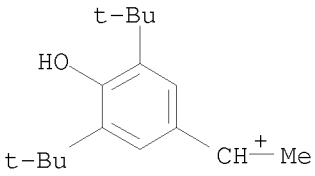


RN 138695-03-1 CAPLUS
CN Phenoxy, 4-[1-[1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2,2-dimethylpropoxy]-2,2-dimethylpropyl]-2,6-bis(1,1-dimethylethyl)-, (R*,S*)-(9CI) (CA INDEX NAME)

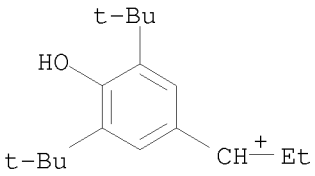
Relative stereochemistry.



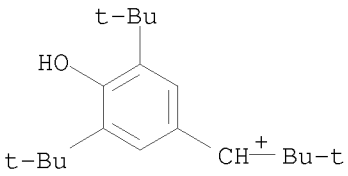
IT 138694-85-6P 138694-95-8P 138695-00-8P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and reactions of)
RN 138694-85-6 CAPLUS
CN Ethylium, 1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]- (9CI) (CA INDEX NAME)



RN 138694-95-8 CAPLUS
CN Propylium, 1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]- (9CI) (CA INDEX NAME)



RN 138695-00-8 CAPLUS
CN Propylium, 1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2,2-dimethyl-(9CI) (CA INDEX NAME)



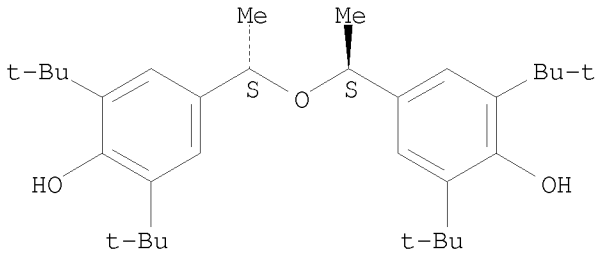
IT 138694-86-7P 138694-87-8P 138694-90-3P
138694-91-4P 138694-96-9P 138694-97-0P
138695-01-9P 138721-75-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 138694-86-7 CAPLUS

CN Phenol, 4,4'-(oxydiethylidene)bis[2,6-bis(1,1-dimethylethyl)-, (R*,R*)-(9CI) (CA INDEX NAME)

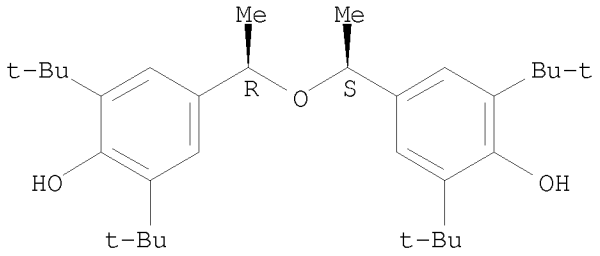
Relative stereochemistry.



RN 138694-87-8 CAPLUS

CN Phenol, 4,4'-(oxydiethylidene)bis[2,6-bis(1,1-dimethylethyl)-, (R*,S*)-(9CI) (CA INDEX NAME)

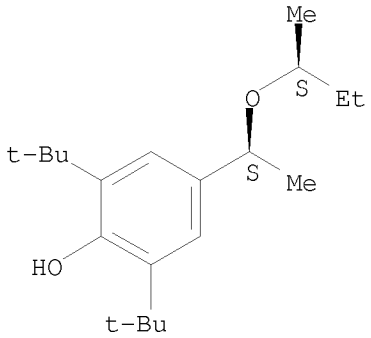
Relative stereochemistry.



RN 138694-90-3 CAPLUS

CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[(1R)-1-[(1R)-1-methylpropoxy]ethyl]-, rel- (CA INDEX NAME)

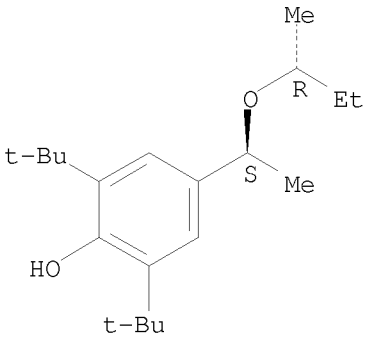
Relative stereochemistry.



RN 138694-91-4 CAPLUS

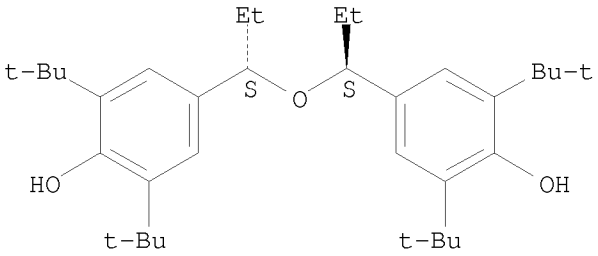
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[(1R)-1-[(1S)-1-methylpropoxy]ethyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



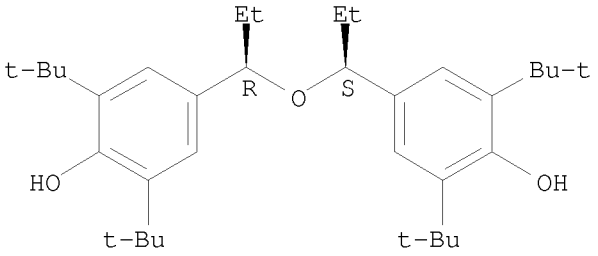
RN 138694-96-9 CAPLUS
CN Phenol, 4,4'-(oxydipropylidene)bis[2,6-bis(1,1-dimethylethyl)-, (R*,R*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



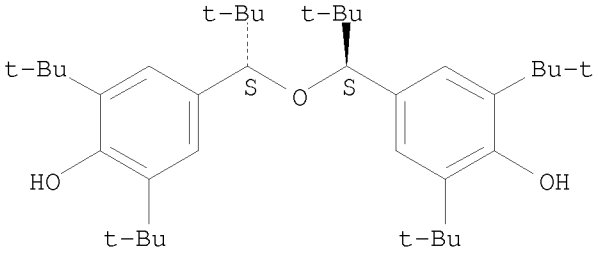
RN 138694-97-0 CAPLUS
CN Phenol, 4,4'-(oxydipropylidene)bis[2,6-bis(1,1-dimethylethyl)-, (R*,S*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



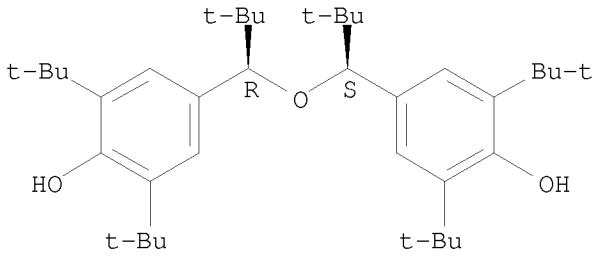
RN 138695-01-9 CAPLUS
CN Phenol, 4,4'-[oxybis(2,2-dimethylpropylidene)]bis[2,6-bis(1,1-dimethylethyl)-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

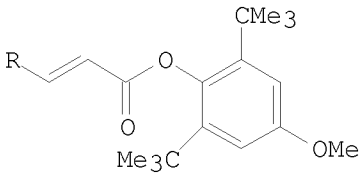


RN 138721-75-2 CAPLUS
CN Phenol, 4,4'-[oxybis(2,2-dimethylpropylidene)]bis[2,6-bis(1,1-dimethylethyl)-, (R*,S*)- (9CI) (CA INDEX NAME)

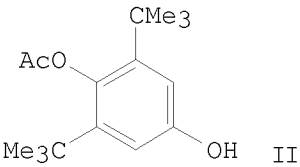
Relative stereochemistry.



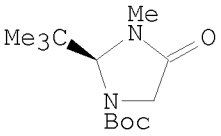
L5 ANSWER 34 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:84124 CAPLUS
DOCUMENT NUMBER: 116:84124
ORIGINAL REFERENCE NO.: 116:14351a,14354a
TITLE: threo-3-Alkyl- and -arylglutamic acid derivatives by Michael additions of Boc-BMI Li-enolates to 2,6-di-tert-butyl-4-methoxyphenyl alkenoates on the diastereoselectivity of the coupling of trigonal centers involving heterocyclic Li-enolates
AUTHOR(S): Suzuki, Keisuke; Seebach, Dieter
CORPORATE SOURCE: Lab. Org. Chem., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
SOURCE: Liebigs Annalen der Chemie (1992), (1), 51-61
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:84124
GI



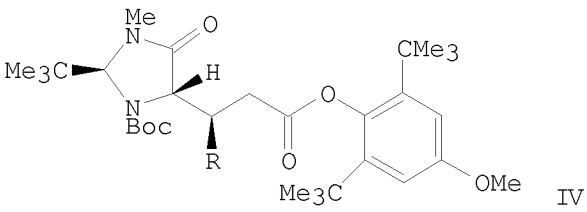
I



II



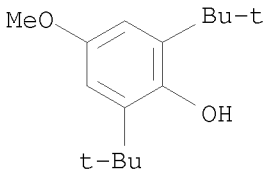
III



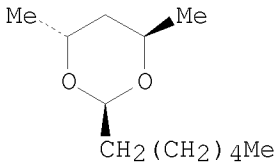
IV

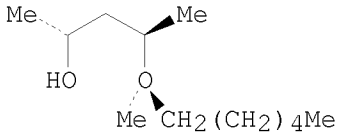
AB Title alkenoates I (R = Me, Et, CHMe2, Ph) were prepared by the aldol condensation of aldehyde RCHO with aryl acetate II in the presence of LDA. The Michael addition reaction of I with the Li enolate of imidazolidinone III (Boc = Me3CO2C) gave glutamate derivs. IV (R = same) with high diastereoselectivity.
IT 489-01-0
RL: RCT (Reactant); RACT (Reactant or reagent)

(acetylation of)
RN 489-01-0 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-methoxy- (CA INDEX NAME)

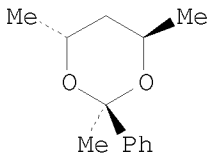


L5 ANSWER 35 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:535480 CAPLUS
DOCUMENT NUMBER: 115:135480
ORIGINAL REFERENCE NO.: 115:23211a,23214a
TITLE: Highly selective acetal cleavage using new organoaluminum reagents
AUTHOR(S): Ishihara, Kazuaki; Hanaki, Naoyuki; Yamamoto, Hisashi
CORPORATE SOURCE: Dep. Appl. Chem., Nagoya Univ., Chikusa, 464-01, Japan
SOURCE: Journal of the American Chemical Society (1991), 113(18), 7074-5
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:135480
GI

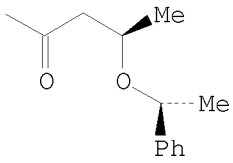




II



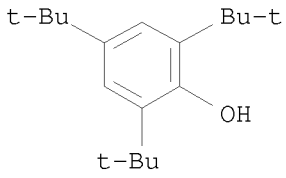
III



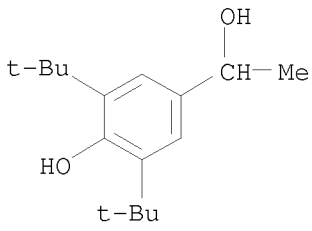
IV

AB Chiral acetals derived from (-)-(2R,4R)-2,4-pentanediol are cleaved selectively by new organoaluminum reagents prepared from trialkylaluminum and halophenols such as pentafluorophenol and 2,4,6-trichlorophenol. The reaction proceeds via a retentive alkylation process which is almost 100% stereoselective in most cases. Thus, dioxane I was added to a solution of Me3Al and C6F5OH in PhMe at 25° to give 70% alkoxypentanol II with >99:1 selectivity. Combined use of Et2AlF and C6F5OH produced a new catalyst for an intramol. Meerwein-Ponndorf-Verley-Oppenauer reaction and acetals, e.g., III, were converted to β-alkoxy ketones, e.g., IV, efficiently and selectively.
IT 732-26-3, 2,4,6-Tri-tert-butylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(conversion into aryloxydialkylaluminum and stereoselective ring cleavage-alkylation with, of chiral cyclic acetals)

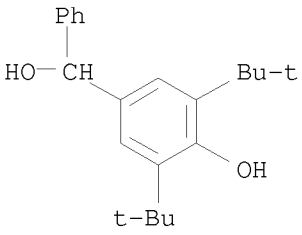
RN 732-26-3 CAPLUS
CN Phenol, 2,4,6-tris(1,1-dimethylethyl)- (CA INDEX NAME)



L5 ANSWER 36 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:514536 CAPLUS
DOCUMENT NUMBER: 113:114536
ORIGINAL REFERENCE NO.: 113:19395a,19398a
TITLE: Chiral recognition of diastereomeric esters and acetals by EPR and NMR investigations
AUTHOR(S): Maeurer, Manfred; Stegmann, Hartmut B.
CORPORATE SOURCE: Inst. Org. Chem., Univ. Tuebingen, Tuebingen, D-7400, Germany
SOURCE: Chemische Berichte (1990), 123(8), 1679-85
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:114536
GI For diagram(s), see printed CA Issue.
AB The reaction of the racemic phenols I (R = Ph, Me) with chiral auxiliaries like PhCHEtCOCl and particularly the lactols (+)-II and (-)-III (Noe's reagent) leads to diastereomeric esters and acetals. The products can be synthesized either in the EPR sample tube or under preparative conditions with subsequent separation of the diastereomers by chromatog. methods. Oxidation of the phenols with PbO_2 in inert solvents provides the corresponding phenoxyls, which are investigated by EPR and ENDOR spectroscopy. The most striking features of these spectra are the differences in the β-proton coupling consts. of up to several Gauss, indicating a significant alteration of the hyperconjugation angle. These results are interpreted in terms of the population of specific conformations favored by stereoelectronic and steric interactions, which are confirmed by careful investigations of the shielding and deshielding effects in the 1H-NMR spectra of the corresponding phenols.
IT 14681-20-0 20017-39-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(acetalization and esterification of, diastereoisomers from)
RN 14681-20-0 CAPLUS
CN Benzenemethanol, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl- (CA INDEX NAME)

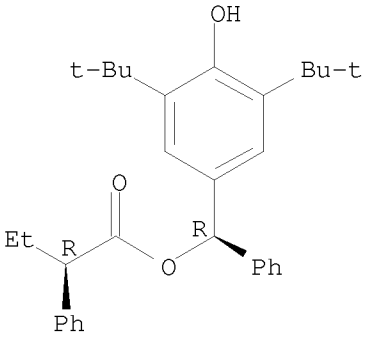


RN 20017-39-4 CAPLUS
CN Benzenemethanol, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-phenyl- (CA INDEX NAME)



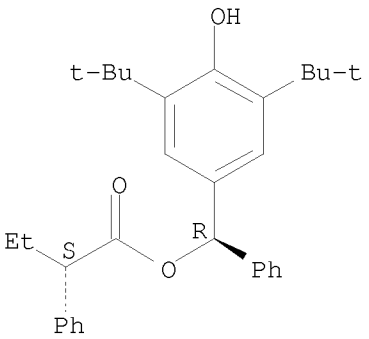
IT 126504-48-1P 126504-49-2P 126504-50-5P
126504-51-6P 126504-56-1P 126504-57-2P
126504-58-3P 126638-18-4P 126638-19-5P
126638-20-8P 126638-21-9P 126638-22-0P
126640-48-0P 126640-49-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, NMR and oxidation of)
RN 126504-48-1 CAPLUS
CN Benzeneacetic acid, α-ethyl-,
(R)-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]phenylmethyl ester,
(αR)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 126504-49-2 CAPLUS
CN Benzeneacetic acid, α-ethyl-,
(R)-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]phenylmethyl ester,
(αS)-rel- (CA INDEX NAME)

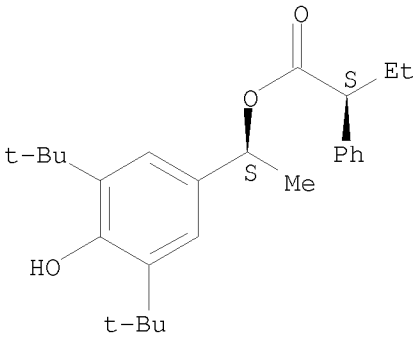
Relative stereochemistry.



RN 126504-50-5 CAPLUS
CN Benzeneacetic acid, α-ethyl-,

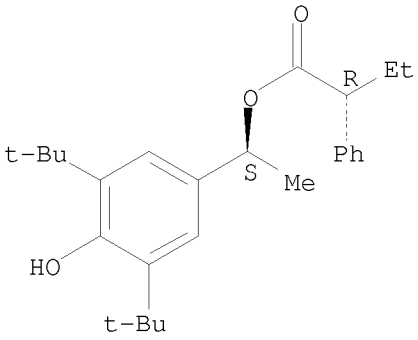
(1R)-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]ethyl ester,
(αR)-rel- (CA INDEX NAME)

Relative stereochemistry.



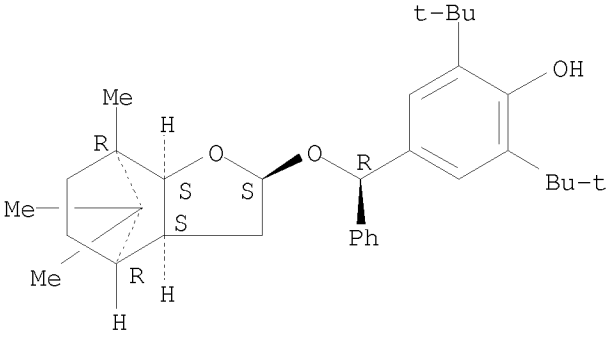
RN 126504-51-6 CAPLUS
CN Benzeneacetic acid, α-ethyl-,
(1R)-1-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]ethyl ester,
(αS)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 126504-56-1 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]phenylmethyl]-,
[2S-[2α(S*),3aβ,4β,7β,7aβ]]- (9CI) (CA INDEX NAME)

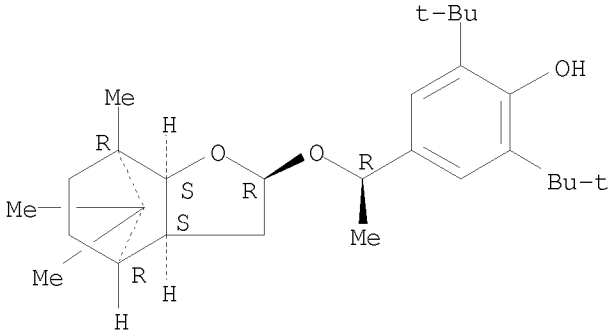
Absolute stereochemistry.



RN 126504-57-2 CAPLUS

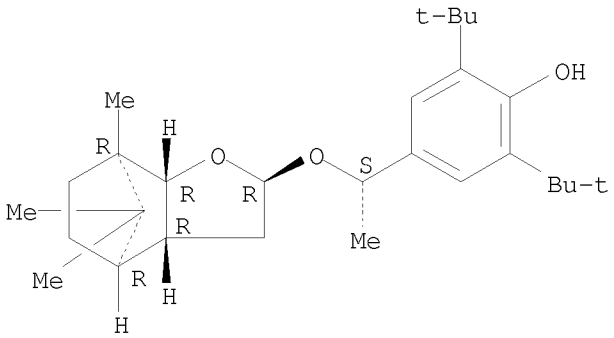
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[1-[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]ethyl]-, [2R-[2α(R*),3aβ,4β,7β,7aβ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



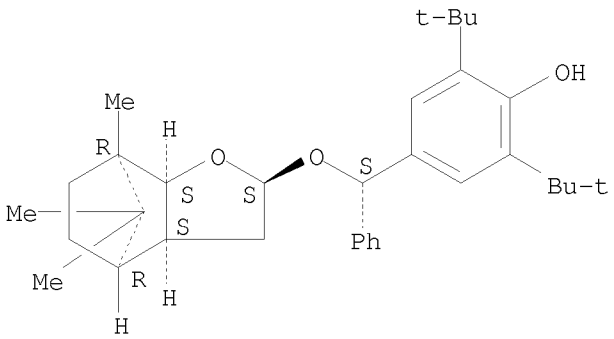
RN 126504-58-3 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[1-[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]ethyl]-, [2R-[2α(S*),3aα,4β,7β,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



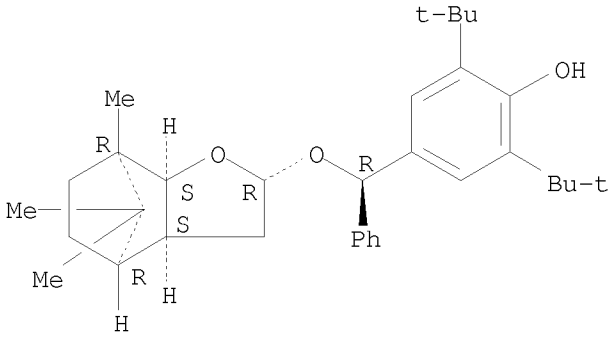
RN 126638-18-4 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]phenylmethyl]-, [2S-[2α(R*),3aβ,4β,7β,7aβ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



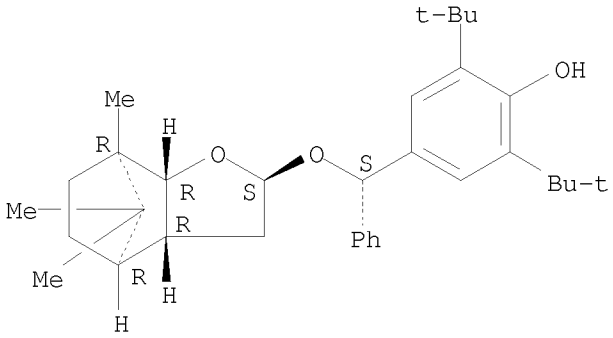
RN 126638-19-5 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]phenylmethyl]-, [2R-[2α(R*),3aα,4α,7α,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



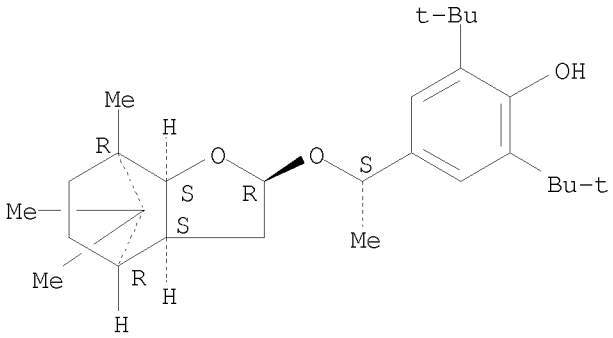
RN 126638-20-8 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]phenylmethyl]-, [2S-[2α(R*),3aα,4β,7β,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



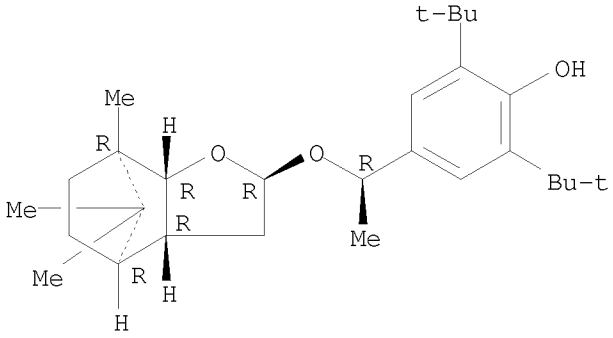
RN 126638-21-9 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[1-[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]ethyl]-, [2R-[2α(S*),3aβ,4β,7β,7aβ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



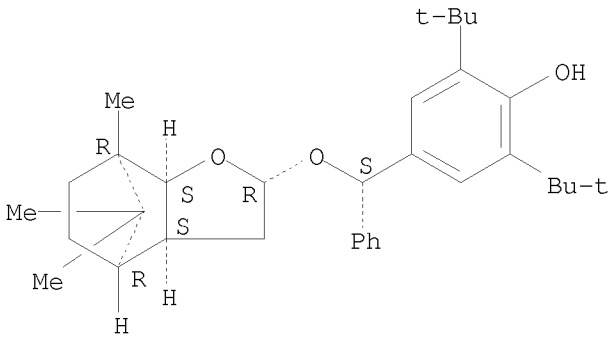
RN 126638-22-0 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[1-[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]ethyl]-, [2R-[2α(R*),3aα,4β,7β,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



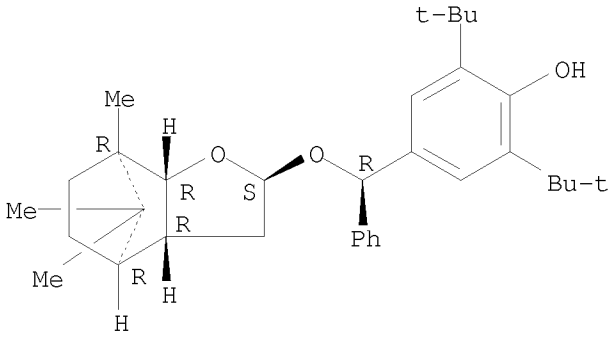
RN 126640-48-0 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]phenylmethyl]-, [2R-[2α(S*),3aα,4α,7α,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

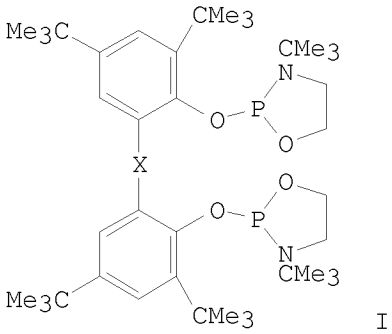


RN 126640-49-1 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[[(octahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2-yl)oxy]phenylmethyl]-, [2S-[2α(S*),3aα,4β,7β,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 37 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:529162 CAPLUS
DOCUMENT NUMBER: 109:129162
ORIGINAL REFERENCE NO.: 109:21529a,21532a
TITLE: Sterically congested molecules: synthesis, characterization, and unique spectral characteristics of hexa-tert-butyl-substituted biaryl bis(1,3,2-oxazaphospholidines)
AUTHOR(S): Pastor, Stephen D.; Hyun, James L.; Odorisio, Paul A.; Rodebaugh, Ronald K.
CORPORATE SOURCE: Addit. Div., Ciba-Geigy Corp., Ardsley, NY, 10502, USA
SOURCE: Journal of the American Chemical Society (1988), 110(19), 6547-55
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:129162
GI



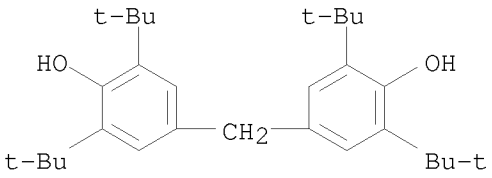
I

AB Title compds. such as I (X = a bond) (II) and I (X = CHMe) (III) were prepared by the reaction of 3-tert-butyl-2-chloro-1,3,2-oxazaphospholidine with sterically hindered Na phenolates. In the solid state, the crystallog. data showed that the P atoms in II and III are chemical nonequiv. This is due to steric interactions within II and III. In II, the aryl-aryl C-C single bond length (1.511 Å) is longer than that expected for a sp2-sp2 single bond (1.48 Å). II represents the 1st fully characterized example in the literature of a mol. containing both a chiral axis and 2 chiral P(III) centers. The observed diastereoselectivity and spectral data of I and II are explained on the

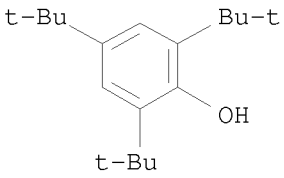
basis of the severe geometric restraints and the resultant mol. asym. that is due to the extreme steric crowding within these mols.

IT 118-82-1 732-26-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorooxazaphospholidines)

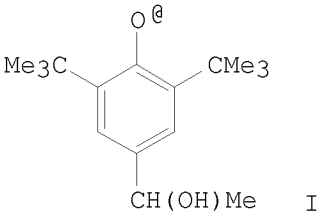
RN 118-82-1 CAPLUS
CN Phenol, 4,4'-methylenebis[2,6-bis(1,1-dimethylethyl)- (CA INDEX NAME)



RN 732-26-3 CAPLUS
CN Phenol, 2,4,6-tris(1,1-dimethylethyl)- (CA INDEX NAME)



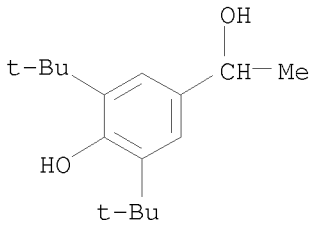
L5 ANSWER 38 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1986:625500 CAPLUS
DOCUMENT NUMBER: 105:225500
ORIGINAL REFERENCE NO.: 105:36395a,36398a
TITLE: Detection of chirality with ENDOR spectroscopy
AUTHOR(S): Stegmann, Hartmut B.; Wendel, Helmut; Hoang Dao Ba; Schuler, Paul; Scheffler, Klaus
CORPORATE SOURCE: Inst. Org. Chem., Univ. Tuebingen, Tuebingen, D-7400, Fed. Rep. Ger.
SOURCE: Angewandte Chemie (1986), 98(11), 988-93
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



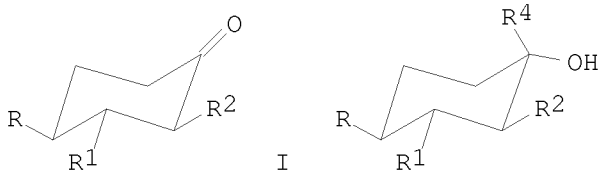
I

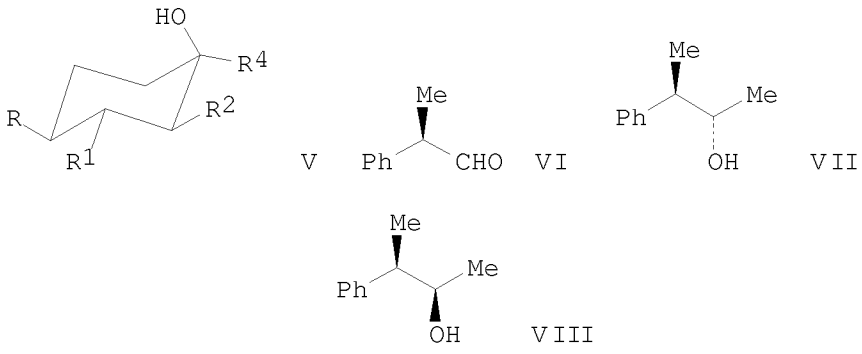
AB The a values for the chiral proton in the (±)-phenoxyl radical I, determined by ENDOR in PhMe or PhMe containing (R)(+)-Me2NCHMePh, were related to the chirality of the proton in each I enantiomer.

IT 14681-20-0
RL: PRP (Properties)
(ENDOR of, chirality in relation to)
RN 14681-20-0 CAPLUS
CN Benzenemethanol, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl- (CA INDEX NAME)



L5 ANSWER 39 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:453724 CAPLUS
DOCUMENT NUMBER: 103:53724
ORIGINAL REFERENCE NO.: 103:8645a,8648a
TITLE: Methylaluminum bis(2,6-di-tert-butyl-4-alkylphenoxide). A new reagent for obtaining unusual equatorial and anti-Cram selectivity in carbonyl alkylation
AUTHOR(S): Maruoka, Keiji; Itoh, Takayuki; Yamamoto, Hisashi
CORPORATE SOURCE: Dep. Appl. Chem., Nagoya Univ., Nagoya, 464, Japan
SOURCE: Journal of the American Chemical Society (1985), 107(15), 4573-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:53724
GI





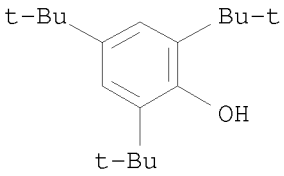
AB A new, stereocontrolled synthesis of equatorial alcs. from cyclohexanones is described, based on the stereoselective activation of the carbonyl moiety by an oxygenophilic Al reagent. Thus, reaction of cyclohexanones I

(R = Me3C, R1 = R2 = H; R = R2 = H, R1 = Me; R = R1 = H, R2 = Me) with MeAl[OC6H2(CMe3)2R3-2,6,4]2 [R3 = Me (II), Me3C (III)] at -78° followed by treatment with organometallics such as R4Li or R4MgBr (R4 = alkyl, alkenyl, alkynyl) gave equatorial alcs. IV exclusively or with axial alcs. V in IV:V ratios of 76-99.5:24-0.5. The II- or III-mediated alkylation was applied to the selective synthesis of hitherto unaccessible anti-Cram alcs. from ordinary α- chiral aldehydes having no ability to be chelated. Thus, methylation of phenylpropionaldehyde VI in presence of III gave alcs. VII and VIII in 93:7 ratio.

IT 732-26-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with trimethylaluminum)

RN 732-26-3 CAPLUS

CN Phenol, 2,4,6-tris(1,1-dimethylethyl)- (CA INDEX NAME)



L5 ANSWER 40 OF 40 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:604234 CAPLUS

DOCUMENT NUMBER: 95:204234

ORIGINAL REFERENCE NO.: 95:34137a,34140a

TITLE: Functional polymers. VII. C(3)-control of stereochemistry in asymmetric reactions catalyzed by polymeric cinchona alkaloids

AUTHOR(S): Kobayashi, Norio; Iwai, Kiyoko

CORPORATE SOURCE: Sagami Chem. Res. Cent., Kanagawa, 229, Japan

SOURCE: Polymer Journal (Tokyo, Japan) (1981), 13(3), 263-71
CODEN: POLJB8; ISSN: 0032-3896

DOCUMENT TYPE: Journal

LANGUAGE: English

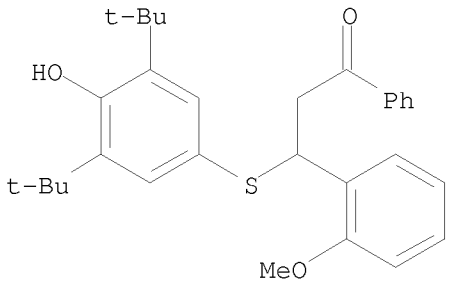
AB Asym. addition of dodecanethiol with β-substituted Ph vinyl ketones were studied using polymeric and monomeric cinchona alkaloids as chiral catalysts. The mode of stereoregulation (C(8), C(9)-control, C(3)-control) varied depending not only on the substituents at C(3) and C(6') of the alkaloid mol. but also on the β-substituent of the unsatd. systems. The C(3)-control was observed when the steric environments of the enantioface differentiating step were sufficiently crowded (combination of polymer catalyst and bulky β-substituent).

IT 79888-35-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 79888-35-0 CAPLUS

CN 1-Propanone, 3-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-3-(2-methoxyphenyl)-1-phenyl-, (+)- (CA INDEX NAME)

Rotation (+).


t-Bu
O
HO
Ph
t-Bu
S
MeO